National Aeronautics and Space Administration

HIGH-END COMPUTING CAPABILITY PORTFOLIO

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NASA Advanced Supercomputing Division

June 10, 2020

NASA HECC Teams Provide COVID-19 Research Support

- HECC is providing supercomputing resources and services to assist researchers in COVID-19 research.
- Four research projects have been awarded supercomputing time on the HECC systems:
  - MIT: “Drug-repurposing for COVID-19 with 3D-aware machine learning,” (GID 79903).
  - NASA Ames: “COVID-19: RNA-seq analysis to identify potential biomarkers indicative of disease severity,” (GID 79902).
  - Virginia Commonwealth University: “Modeling the Dynamic Behavior of Surface Spike Glycoprotein of COVID19 Coronavirus and Designing Biomimetic Therapeutic Compounds,” (GID 79901).
  - NASA Ames: “Whole Genome Analysis Using the NASA Ames Supercomputer to Define Risk Groups for Severe Pulmonary Disease Associated with COVID-19 and Other Illnesses,” (GID 79900).
- HECC support groups have been on-boarding users, assisting in application software support, and providing ongoing production support.

IMPACT: NASA is providing high-end computing resources for COVID-19 studies, as part of the White House Office of Science and Technology Policy COVID-19 High Performance Computing Consortium.

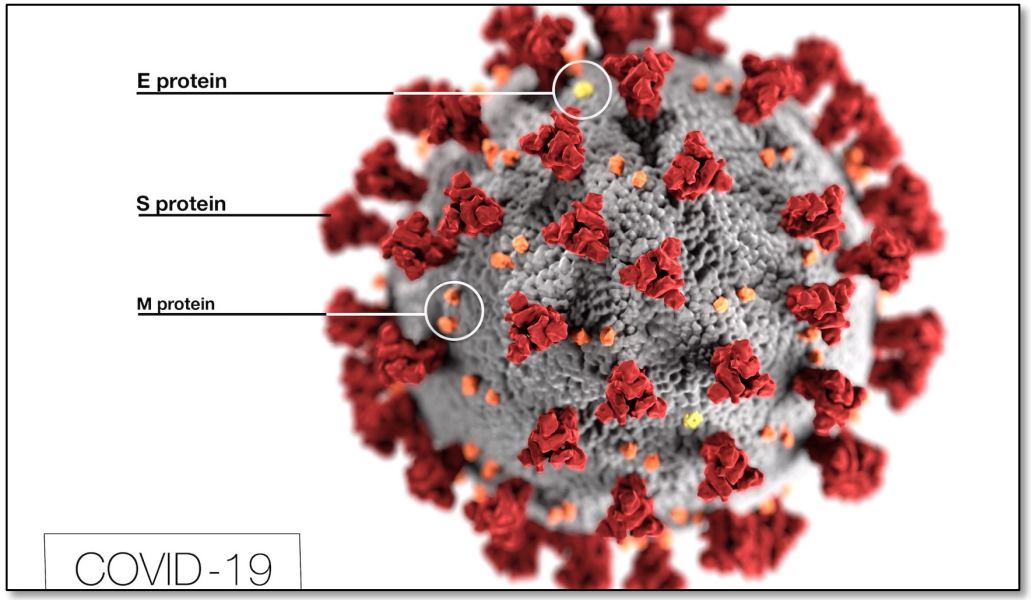
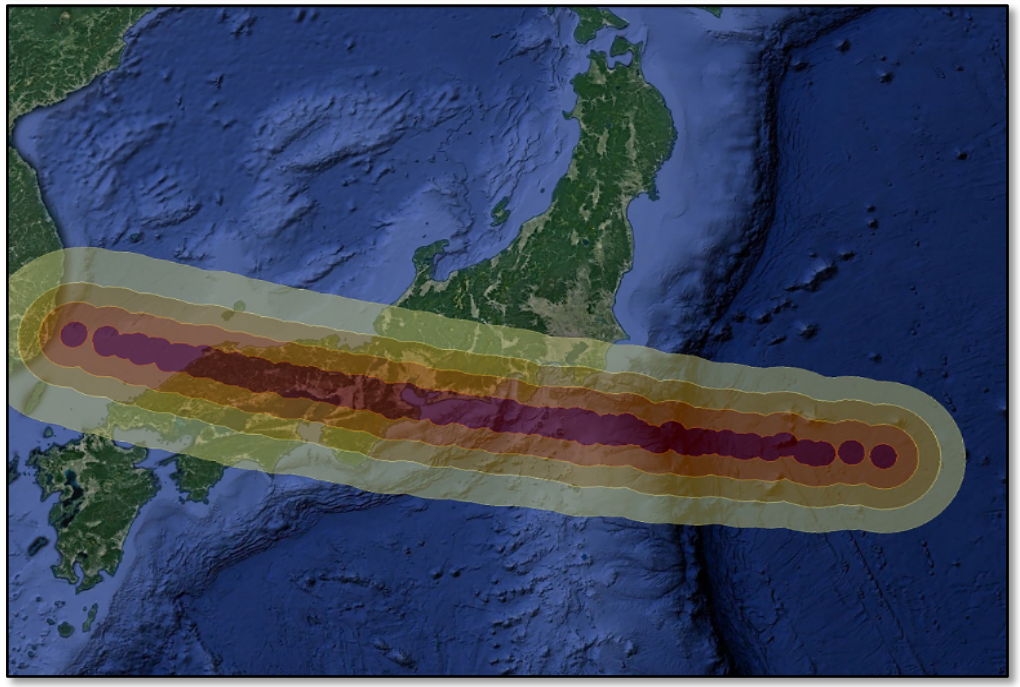


Image depicting coronavirus proteins. *Image credit: CDC*

APP Team Improves Performance of Asteroid Impact Risk Model

- Following on April's improvement to a Python code for NASA's Asteroid Threat Assessment Project (ATAP) group, the HECC Applications Performance and Productivity (APP) team improved performance of ATAP's Probabilistic Asteroid Impact Risk (PAIR) code by a factor of 10 or more.
- PAIR assesses risks due to potential asteroid strikes on Earth by efficiently modeling the entry and damage from millions of hypothetical impact cases. The numbers of people affected by the resulting blast waves, thermal radiation, tsunamis, or large-scale global effects are computed using gridded world population data.
- APP analyzed the code and found several optimization opportunities:
  - Use the Intel icc compiler vs. gcc and enable aggressive in-lining of routines via compilation flags, to improve performance by a factor of 2.5.
  - Reduce the number of distance computations and subdivides of population grid cells to obtain fractional populations falling within damage borders; performance analysis revealed these functions led to many additional expensive operations.
- Based on these findings, the PAIR team revised the search algorithm so that the need for subdivision is greatly reduced, particularly for high-resolution population grids.
- Using a test set of 1 million large (100m-5km) asteroid cases impacting around the world, the new version runs 10 times faster for a low-resolution grid and 30 times faster for a high-resolution grid.

IMPACT: Significant improvements to the PAIR code allow it to run fast enough to use the high-resolution grid, which improves the accuracy of damage predictions for NASA's planetary defense efforts.



Damage zone risk swath from a PAIR simulation of a hypothetical asteroid impact scenario. *Lorien Wheeler, NASA/Ames*

HECC Engineers Enable Singularity Containers Capability

- Engineers on the HECC Systems and Application Performance and Productivity (APP) teams evaluated the functionality and security of Singularity and deployed it for users.
  - Developed by Sylabs Inc., Singularity provides a Docker-like software container capability for shared HPC environments. It allows users to create and have full control of an environment without having to ask system administrators to install anything for them.
  - Users can package their entire scientific workflow, software, and libraries—and even data—into a Singularity container image and use it to run on any platform, including cloud resources, where Singularity is installed.
- To improve security, HECC engineers replaced the method for gaining root privilege offered in the official open-source Singularity version 3.5 release with an in-house option.
  - When building Singularity container images that require root privileges on HECC systems, the Sylabs-provided fakeroot command line option that needs setuid enabled is not allowed.
  - Instead, users can gain root privilege within a container via a HECC-provided fakeroot utility in either one of two NAS-provided base images—CentOS and Ubuntu.
- Guidelines for using the Singularity offering are available through a set of four HECC Knowledge Base articles published in mid-May.

IMPACT: Providing a locally-modified Singularity offering saves the time and effort of both HECC system administrators and users while ensuring security and enabling portability.

```
pfe% singularity exec lolcow which cowsay
/usr/games/cowsay
pfe% singularity exec lolcow cowsay hello
 _______
< hello >
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pfe%
```
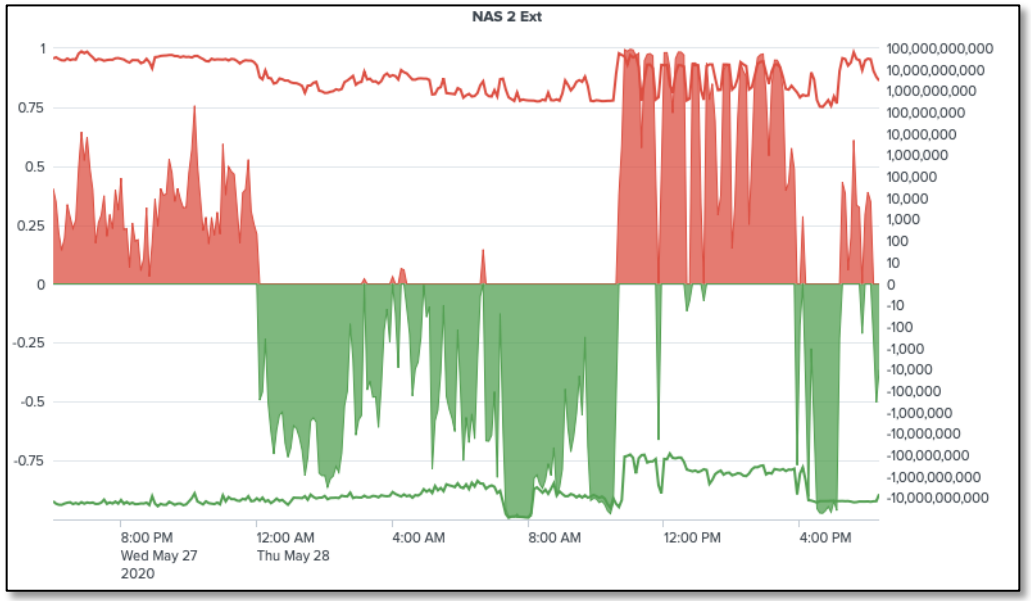

One of several examples of running a popular Singularity test case on Pleiades front ends (PFEs), provided in HECC Knowledge Base articles on Singularity.

New Network Analysis Capabilities Improve HECC Security Monitoring System

- In addition to new features added reported in the April 2020 HECC monthly, security experts added new capabilities to the HECC security monitoring systems. Capabilities include:
  - Better categorization of network flows to improve filtering and increase search performance.
  - Updated Producer-Consumer Ratio (PCR) analysis to be fully interactive, allowing security analysts to remove unwanted data and to drill down to specific time, hosts, ports, and protocols.
  - Improved detection of suspicious network activity that may be signs of compromise.
  - Updated visualizations, with drilldown from network overview to host level activity.
- These increased capabilities provide the Security team with greater insight into network activity that may indicate insider threat activity, data exfiltration, and signs of malware.
- Adds to DNS Analysis Capability Improvements to HECC Security Monitoring System highlighted in April 2020.

IMPACT: New analysis capabilities provide HECC security experts with a unified tool to evaluate network traffic, affording better awareness of the threats and risks to HECC resources.

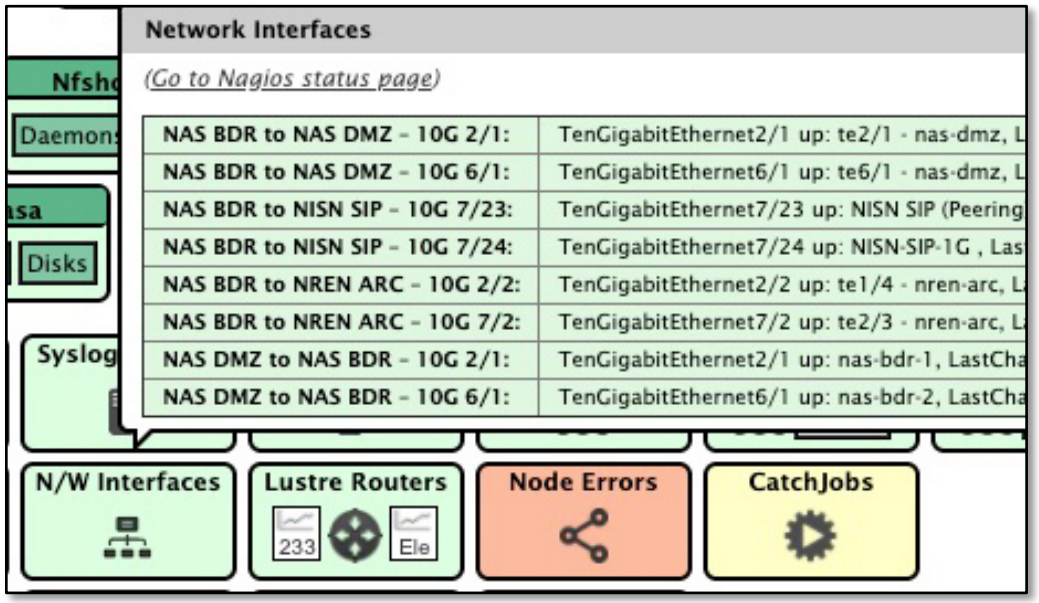


Time series chart from the NAS Situational Awareness System showing Producer-Consumer Ratio (PCR). Red area indicates NAS producing more data than consuming. Green area indicates NAS consuming more data than producing. Red trend line shows amount of data in bytes sent (produced). Green trend line shows amount of data in bytes received (consumed).

Enhanced Network Monitoring for Control Room Staff

- The Networks team augmented the network monitoring capability for Control Room analysts at the NAS facility.
  - Added the status of the NASLAN major network interfaces to the Control Room Heads-Up Display, which enables viewing of uptime, descriptions, device naming, and network traffic.
- This capability increases situational awareness by enabling the Control Room staff to more easily determine if NASLAN equipment is causing a network outage.
  - This feature is in addition to the existing notification alert system for control room staff.
- The Networks team utilized the Nagios network monitoring system that the Tools team already uses to monitor other HECC resources and Mission Assurance System (MAS) servers.

IMPACT: This new network monitoring capability provides a real-time visual representation of the major NASLAN network interfaces and shows relevant information, including uptime, directly on the Control Room Heads-Up Display.



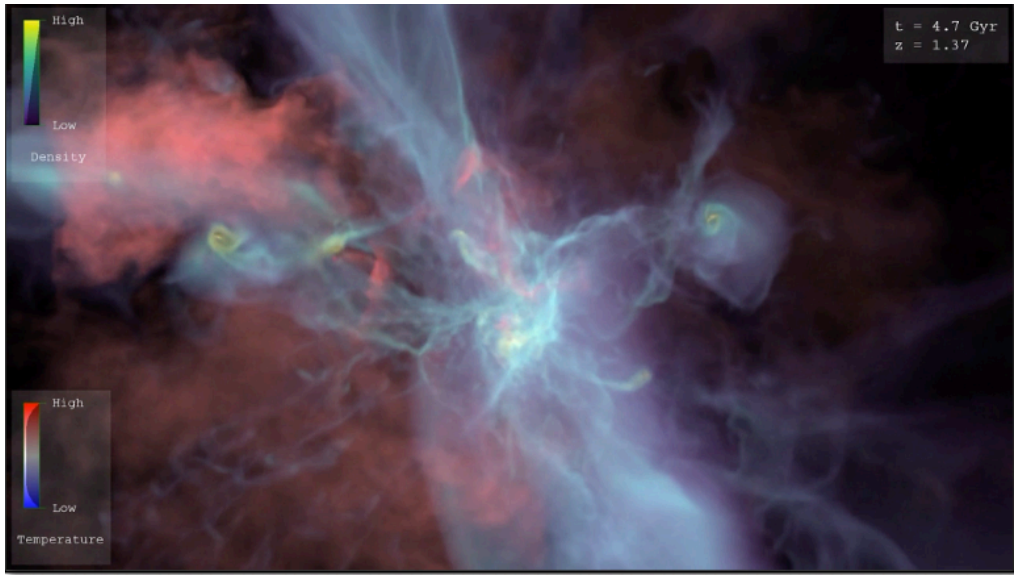
The updated Control Room Heads-Up Display depicts the option to display the status of the NASLAN major network interfaces.

FOGGIE: Simulating the Cosmic Fog Around Galaxies*

- Researchers from the Space Telescope Science Institute and Johns Hopkins University are running cosmological simulations on Pleiades to model how galaxies and gas change through time.
- Using their Enzo cosmological hydrodynamic code, the "Figuring Out Gas & Galaxies In Enzo (FOGGIE)" project scientists model the co-evolution of galaxies and their gas with a focus on resolving the ultra-diffuse circumgalactic medium (CGM) with unprecedented fidelity.
- The simulations reveal a richly structured CGM full of churning turbulent gas, small clouds, and tenuous hot gas. Results are used to help interpret real observations made by NASA's Hubble Space Telescope and other observatories.
  - Hubble observations show that low-ionization gas, which should be relatively cool and have higher density, often has kinematic structure very similar to more highly ionized gas, which is expected to generically be hotter and lower density.
  - The high-fidelity FOGGIE simulations reveal that sometimes the kinematically coincident gas is co-spatial, but often it is not; rather, the observation is a chance superposition along the line of sight.

** HECC provided supercomputing resources and services in support of this work.*

IMPACT: Coupled with observational data from Hubble and other space-based observatories, simulations run on HECC resources help reveal the physics of the dynamic and structurally complex circumgalactic medium—a crucial step to understanding how galaxies form and evolve.



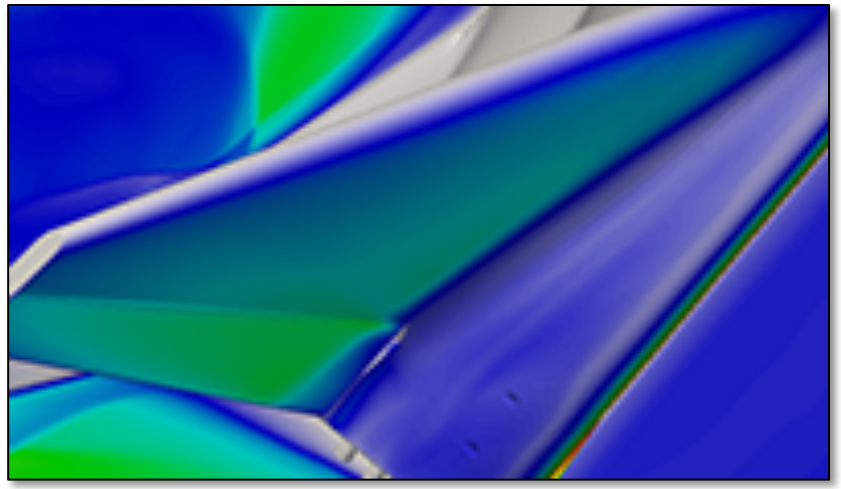
Video from a simulation depicting gas in and around an evolving galaxy across billions of years. Gas density is highest (orange/yellow) at galaxy's center, but the lower-density gas (blue/black) still has complex structure. *Molly S. Peeples, Space Telescope Science Institute/Johns Hopkins University; Chris Henze, NASA Ames*

Simulating Dream Chaser® Spaceplane Aerodynamics*

- Aerodynamics engineers at Sierra Nevada Corporation (SNC) ran CFD simulations on the Pleiades and Endeavour supercomputers to develop aerodynamic and aerothermal preflight databases for SNC's reusable Dream Chaser spacecraft.
  - These databases are used by SNC's Guidance, Navigation and Control for preflight predictions and control analysis and development of the Thermal Protection Systems (TPS) used to protect the vehicle during reentry.
- Using wind tunnel data as anchoring data, the SNC team developed and expanded the Dream Chaser preflight databases using thousands of aerodynamic and aerothermal predictions, and NASA-developed CFD packages, including FUN3D, CART3D, and DPLR (Data Parallel Line Relaxation).
- Access to HECC's computing resources resulted in approximately 20,000 unique high-fidelity CFD simulations to calculate the aerodynamic forces and moments acting on the vehicle, control surface interactions, and aerodynamic increments by firing Reaction Control System thrusters throughout the Entry, Descent, and Landing trajectory.

** HECC provided supercomputing resources and services in support of this work.*

IMPACT: Vital to the success of the Dream Chaser spacecraft is the accurate characterization of aerodynamic forces on the airframe and control surfaces during atmospheric flight. Improvements to spacecraft will benefit NASA's payload capability to and from the International Space Station.



Visualization of the Reaction Control System thruster firing at hypersonic velocities during entry, descent, and landing at various angles of attack of the Dream Chaser spacecraft. As the angle of attack increases, the thruster plume impinges on the wing, changing both the pressure distribution and the vehicle's aerodynamics.
Matt Opgenorth, Sierra Nevada Corporation

Papers

- "**Optical Phase Curve of the Ultra-Hot Jupiter WASP-121b**," V. Bourrier, et al., Astronomy & Astrophysics, vol. 637, published online May 8, 2020. *
  https://www.aanda.org/articles/aa/full_html/2020/05/aa36647-19/aa36647-19.html
- "**Shape and Size of Large-Scale Vortices: A Generic Fluid Pattern in Geophysical Fluid Dynamics**," L.-A. Couston, et al., Physical Review Research, vol. 2, issue 2, May 8, 2020. *
  https://journals.aps.org/prresearch/abstract/10.1103/PhysRevResearch.2.023143
- "**Formation and Evolution of the Large-Scale Magnetic Fields in Venus Ionosphere: Results from a 3D Global Multi-Species MHD Model**," Y. Ma, et al., Geophysical Research Letters, May 10, 2020. *
  https://agupubs.onlinelibrary.wiley.com/doi/abs/10.1029/2020GL087593
- "**An Unusual Transmission Spectrum for the Sub-Saturn KELT-11b Suggestive of a Sub-Solar Water Abundance**," K. Colón, et al., arXiv:2005.05153 [astro-ph.EP], May 11, 2020. *
  https://arxiv.org/abs/2005.05153
- "**Impacts of Aerosol and Environmental Conditions on Maritime and Continental Deep Convective Systems Using a Bin Microphysical Model**," T. Iguchi, et al., Journal of Geophysical Research: Atmospheres, May 12, 2020. *
  https://agupubs.onlinelibrary.wiley.com/doi/abs/10.1029/2019JD030952

** HECC provided supercomputing resources and services in support of this work*

Papers (cont.)

- "**Plasma Characterization at Comet 67P between 2 and 4 AU from the Sun with the RPC-MIP Instrument**," G. Wattieaux, et al., Astronomy & Astrophysics, May 12, 2020. * https://www.aanda.org/articles/aa/pdf/forth/aa37571-20.pdf
- "**The Confinement of the Heliosheath Plasma by the Solar Magnetic Field as Revealed by Energetic Neutral Atom Simulations**," M. Kornbleuth, et al., arXiv:2005.06643 [astro-ph.SR], May 13, 2020. * https://arxiv.org/abs/2005.06643
- "**High-Order Gas-Kinetic Scheme with Parallel Computation for Direct Numerical Simulation of Turbulent Flows**," G. Cao, L. Pan, K. Xu, arXiv:2005.08736 [physics.comp-ph], May 15, 2020. * https://arxiv.org/abs/2005.08736
- "**PTFO 8-8695: Two Stars, Two Signals, No Planet**," L. Bouma, et al., arXiv:2005.10253 [astro-ph.SR], May 20, 2020. * https://arxiv.org/abs/2005.10253
- "**Tuning the Exospace Weather Radio for Stellar Coronal Mass Ejections**," J. Alvarado-Gómez, et al., The Astrophysical Journal, vol. 895, no. 1, May 22, 2020. * https://iopscience.iop.org/article/10.3847/1538-4357/ab88a3
- "**Estimation of Key Sunquake Parameters through Hydrodynamic Modeling and Cross-Correlation Analysis**," J. Stephan, A. Kosovichev, The Astrophysical Journal, vol. 895, no. 1, May 26, 2020. * https://iopscience.iop.org/article/10.3847/1538-4357/ab88ae

** HECC provided supercomputing resources and services in support of this work*

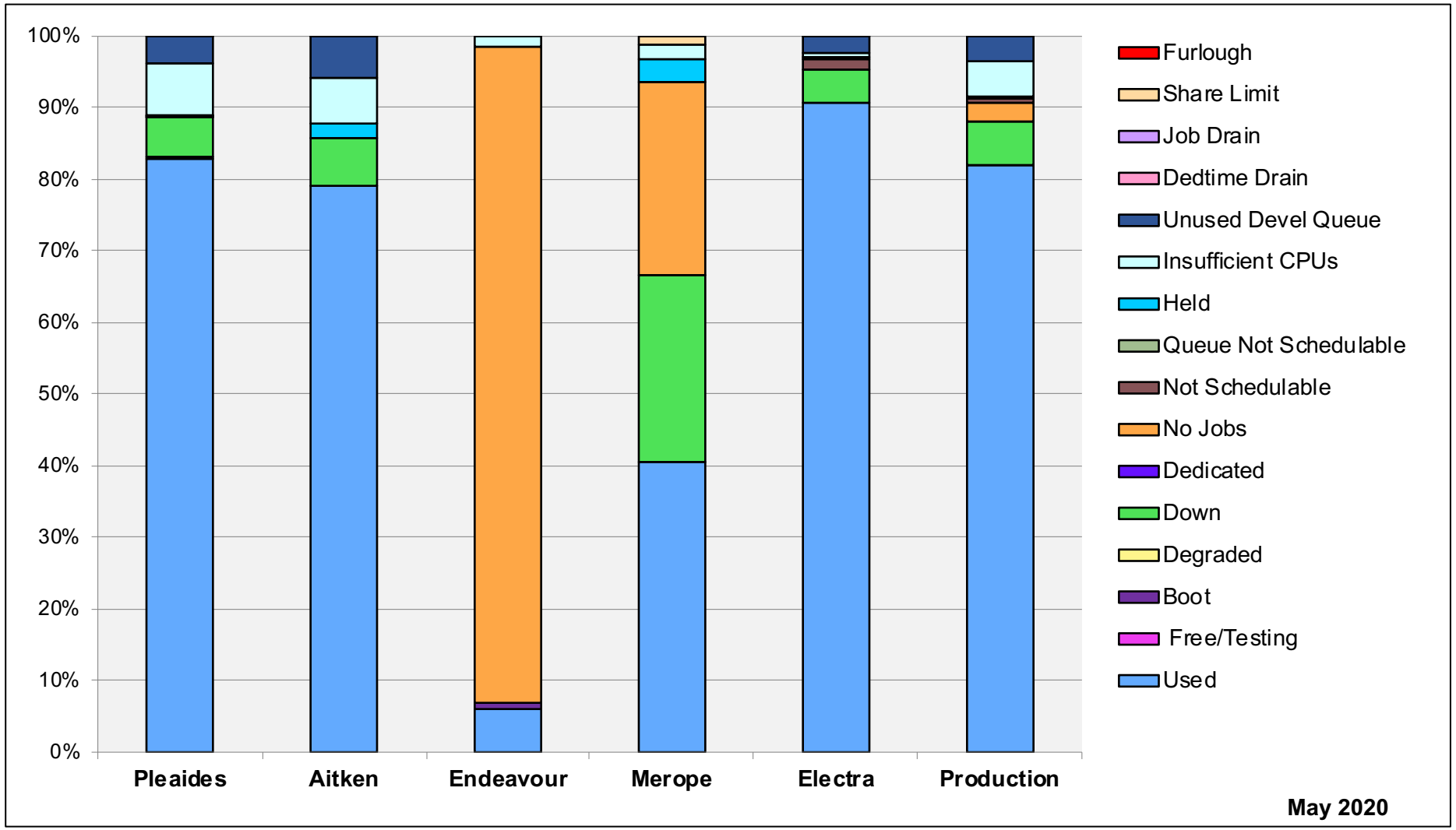
News and Events

- **NASA Supercomputers Power COVID-19 Research**, *NASA Feature,* May 29, 2020—NASA is flexing its supercomputing muscle to help crack some of the most pressing questions surrounding COVID-19, from basic science on how the virus interacts with cells in the human body to genetic risk factors to screening for potential therapeutic drugs. https://www.nasa.gov/feature/esd/2020/nasa-supercomputers-power-covid-19-research
- **NASA is Asking Gamers and Citizen Scientists to Help Map the World's Corals**, *World Economic Forum,* May 26, 2020—America's National Aeronautics and Space Administration has called upon ordinary people to help them map the world's coral. (Re-post of NASA Ames blog on April 29, 2020.) https://www.weforum.org/agenda/2020/05/nasa-science-coral-oceans-floor-explore-civilians-exploration
- **NAS Researchers Bring Asteroid Simulation Down to Earth**, *NASA Advanced Supercomputing Division Feature*, May 1, 2020—Millions of hypothetical impact and airburst scenarios simulated on NASA supercomputers are helping researchers develop the modeling tools we'll need if a real asteroid threat is ever identified. https://www.nas.nasa.gov/publications/articles/feature_asteroid_threat_assessment_part_1.html

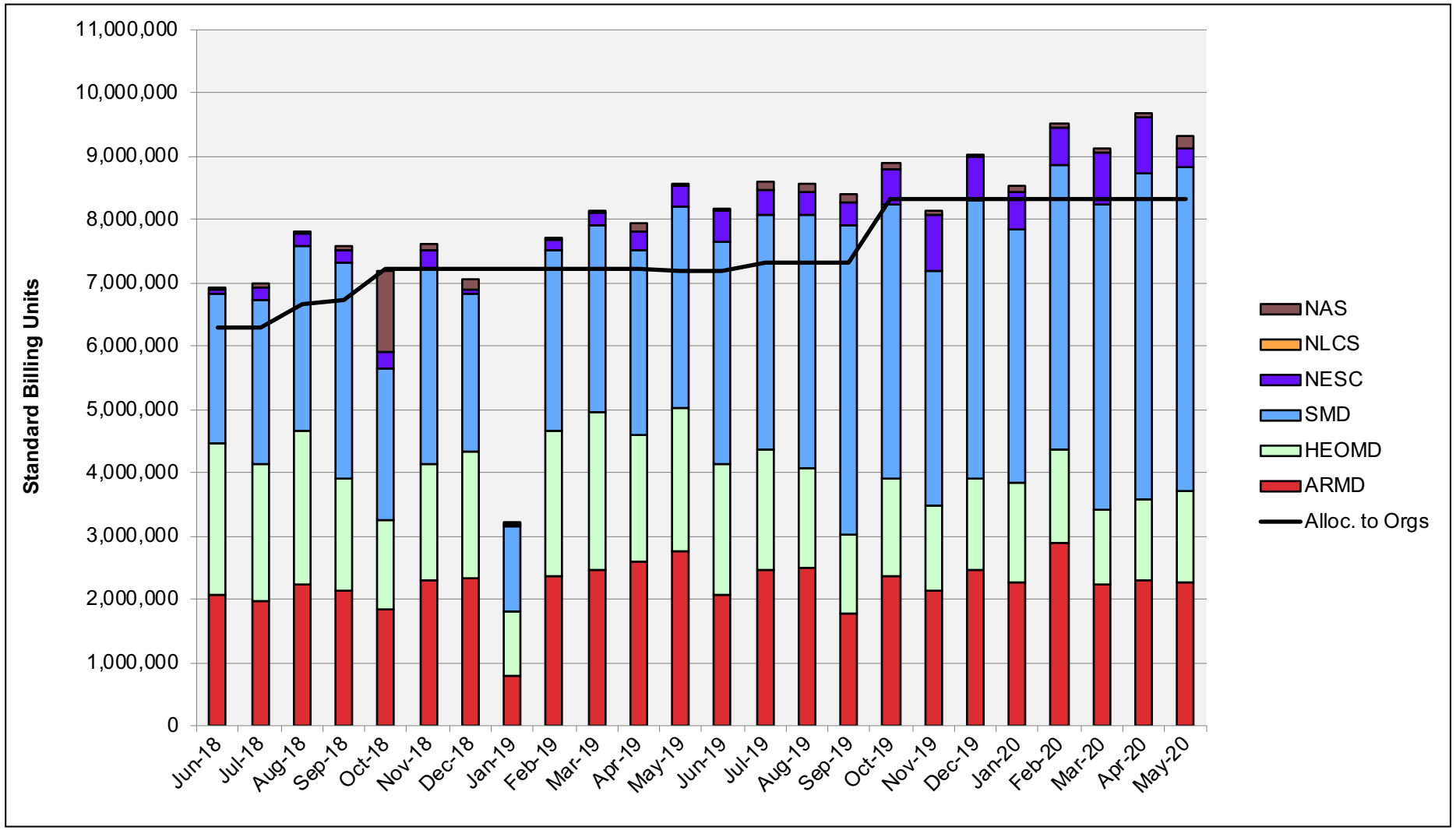
News and Events: Social Media

- **Coverage of NAS Stories**
  - Asteroid Threat Assessment Feature Story:
    - NAS: Twitter 6 retweets, 16 likes
    - NASA Supercomputing: Facebook 301 users reached, 45 engagements, 13 likes, 5 shares
  - Drone Aeroacoustics SC Demo:
    - NAS: Twitter 5 retweets, 9 likes
    - NASA Supercomputing: Facebook 1,376 users reached, 169 engagements, 21 likes, 12 shares

HECC Utilization



HECC Utilization Normalized to 30-Day Month



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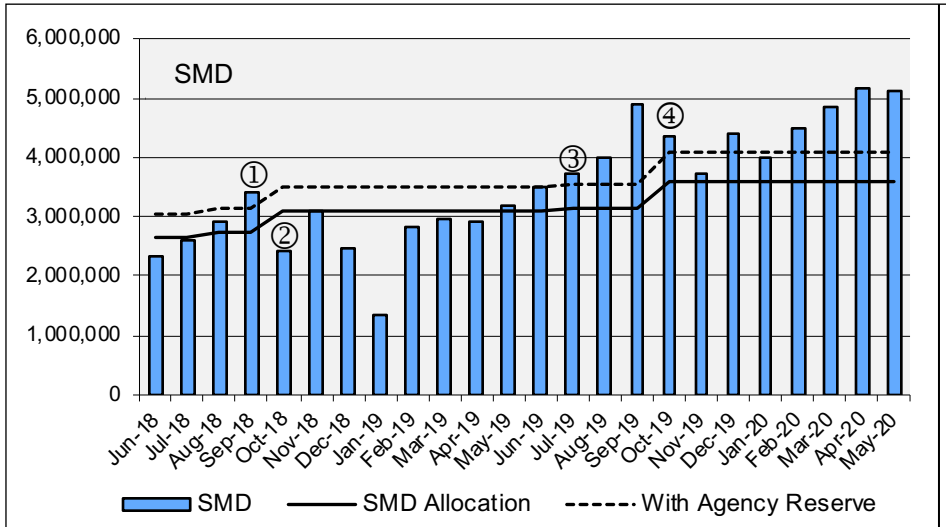
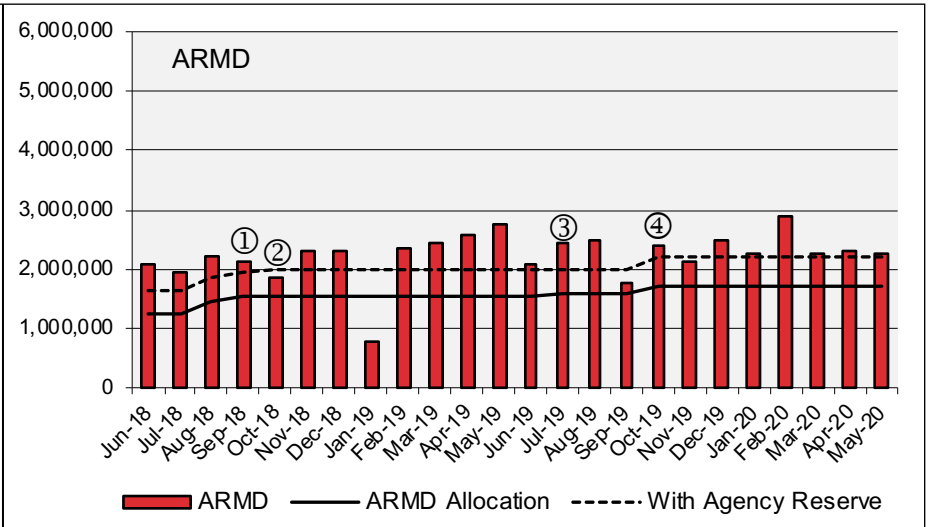
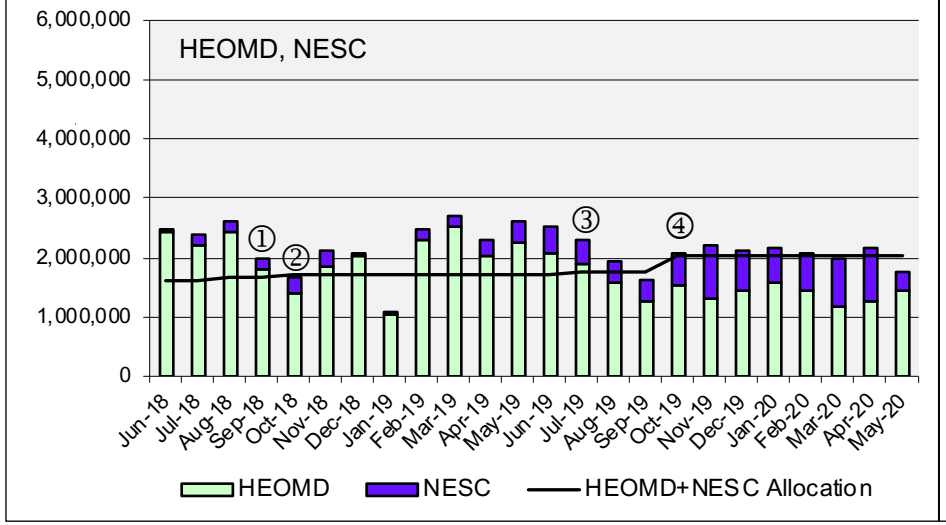






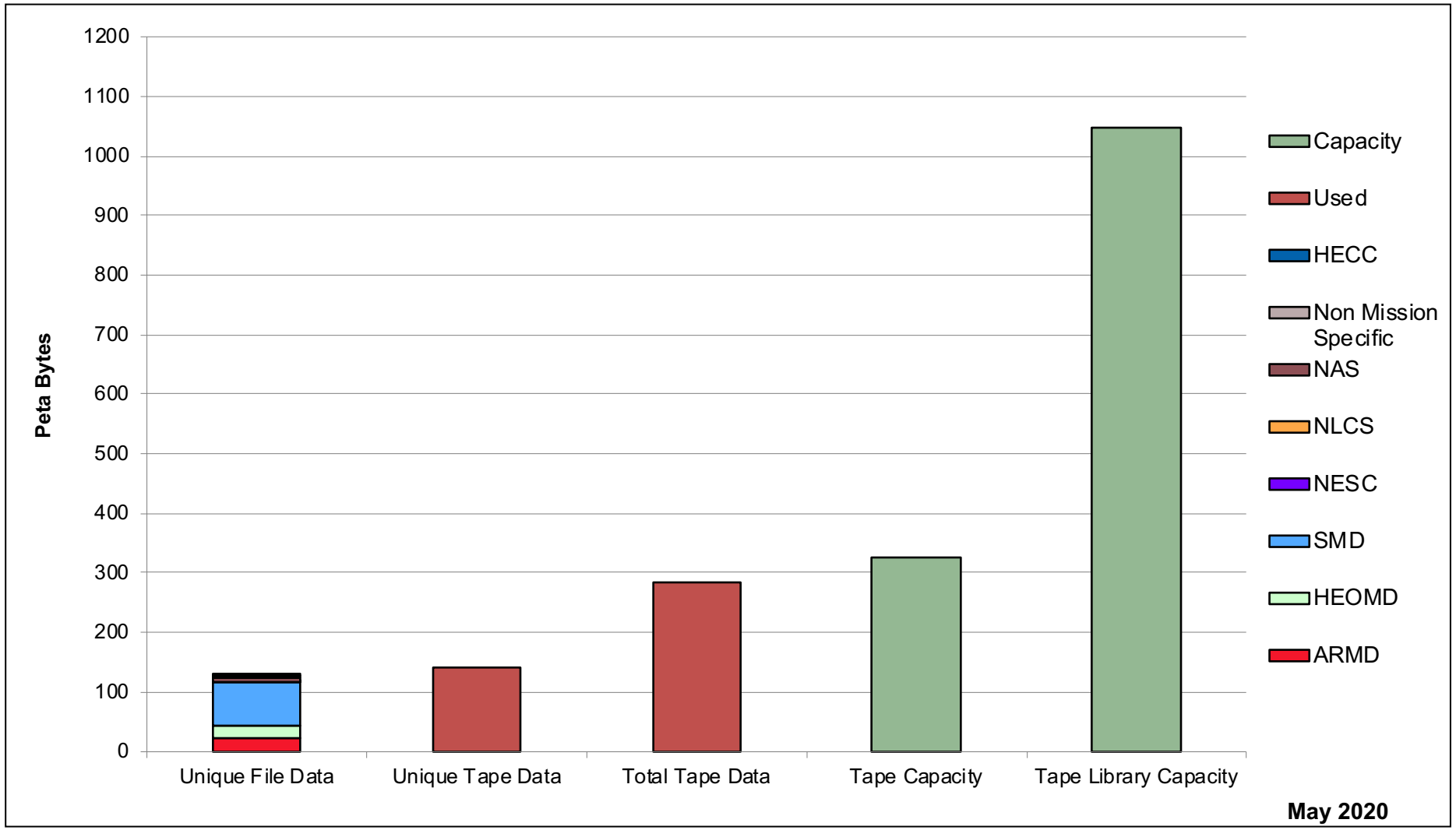
① 4 Skylake E cells (16 D Rack Equivalence) added to Electra

② 2 Skylake E cells (8 D Rack Equivalence) added to Electra; 1 rack is dedicated to ARMD

③ 2 Skylake E cells (8 D Rack Equivalence) added to Electra; 1 rack is dedicated to SMD

④ Skylake Tesla GPU V100 Nodes installed

Tape Archive Status



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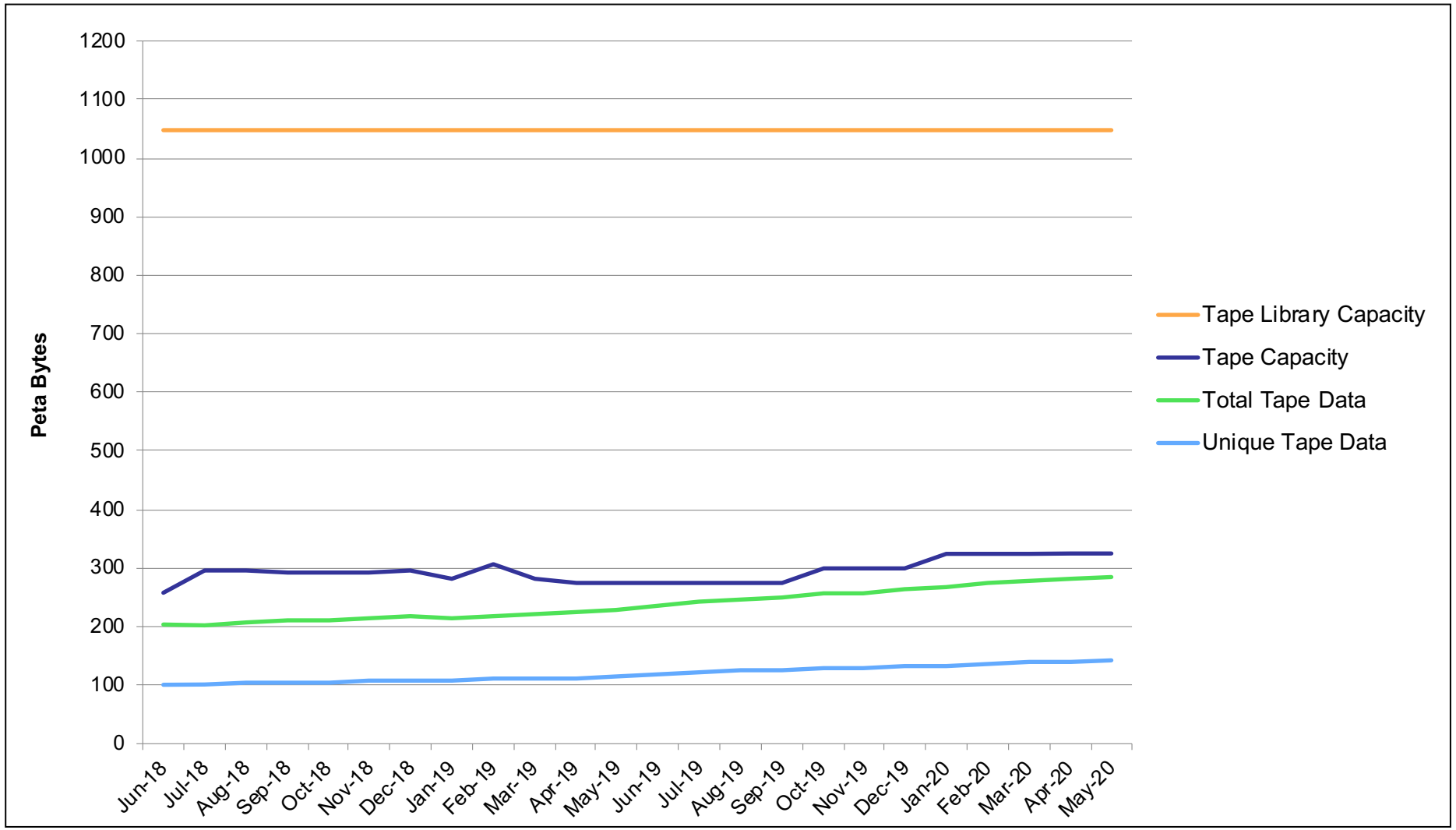
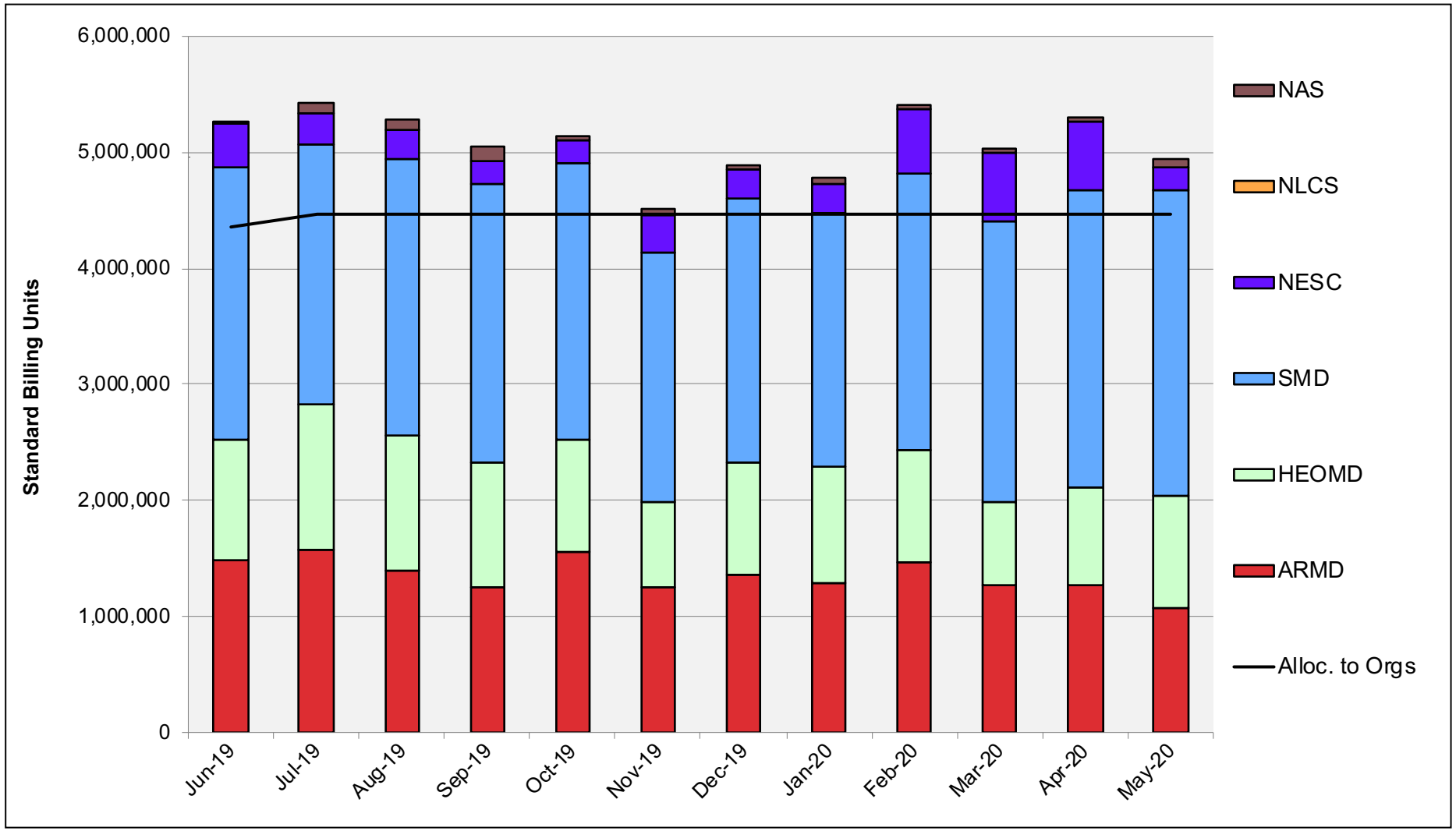
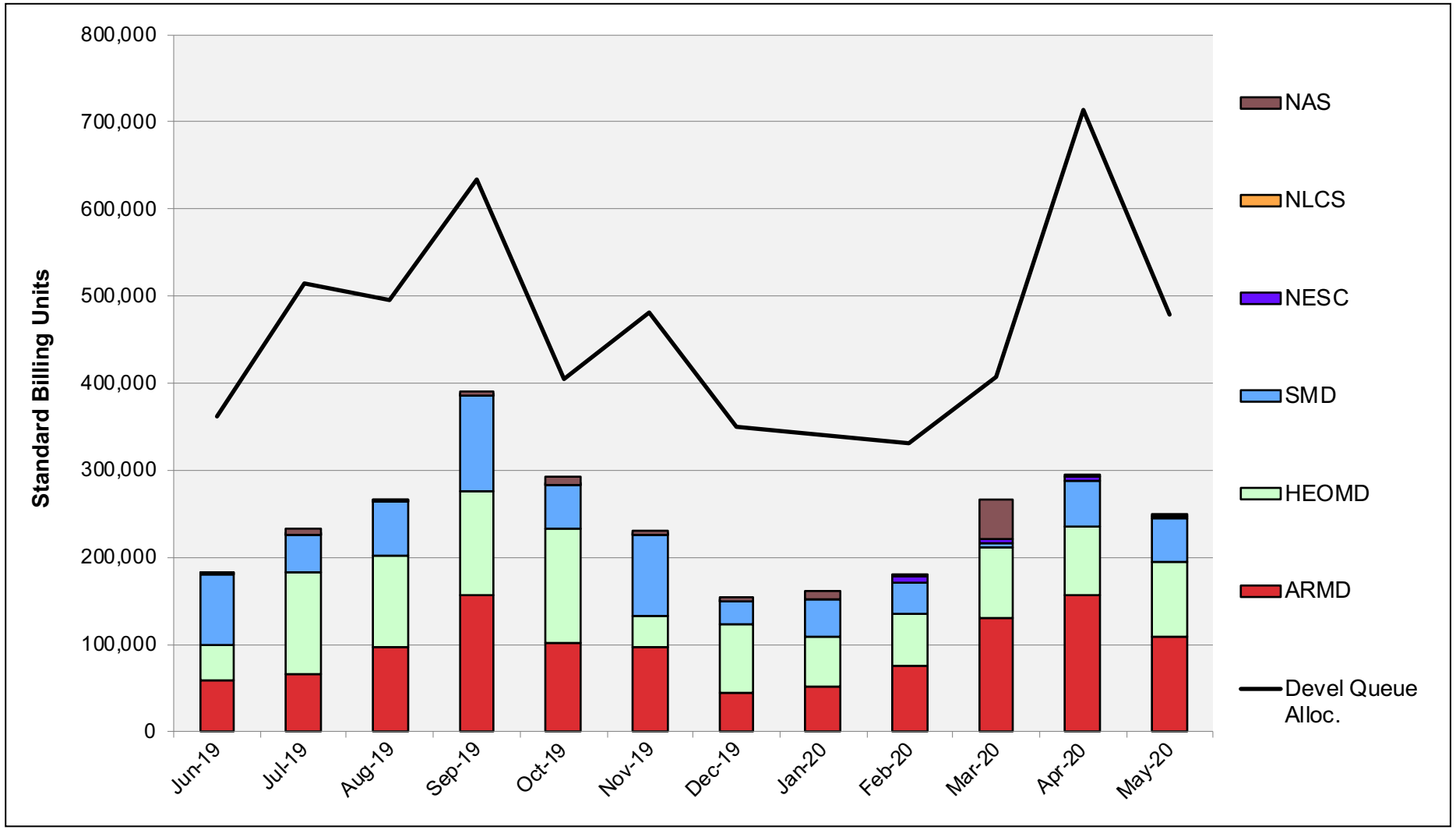


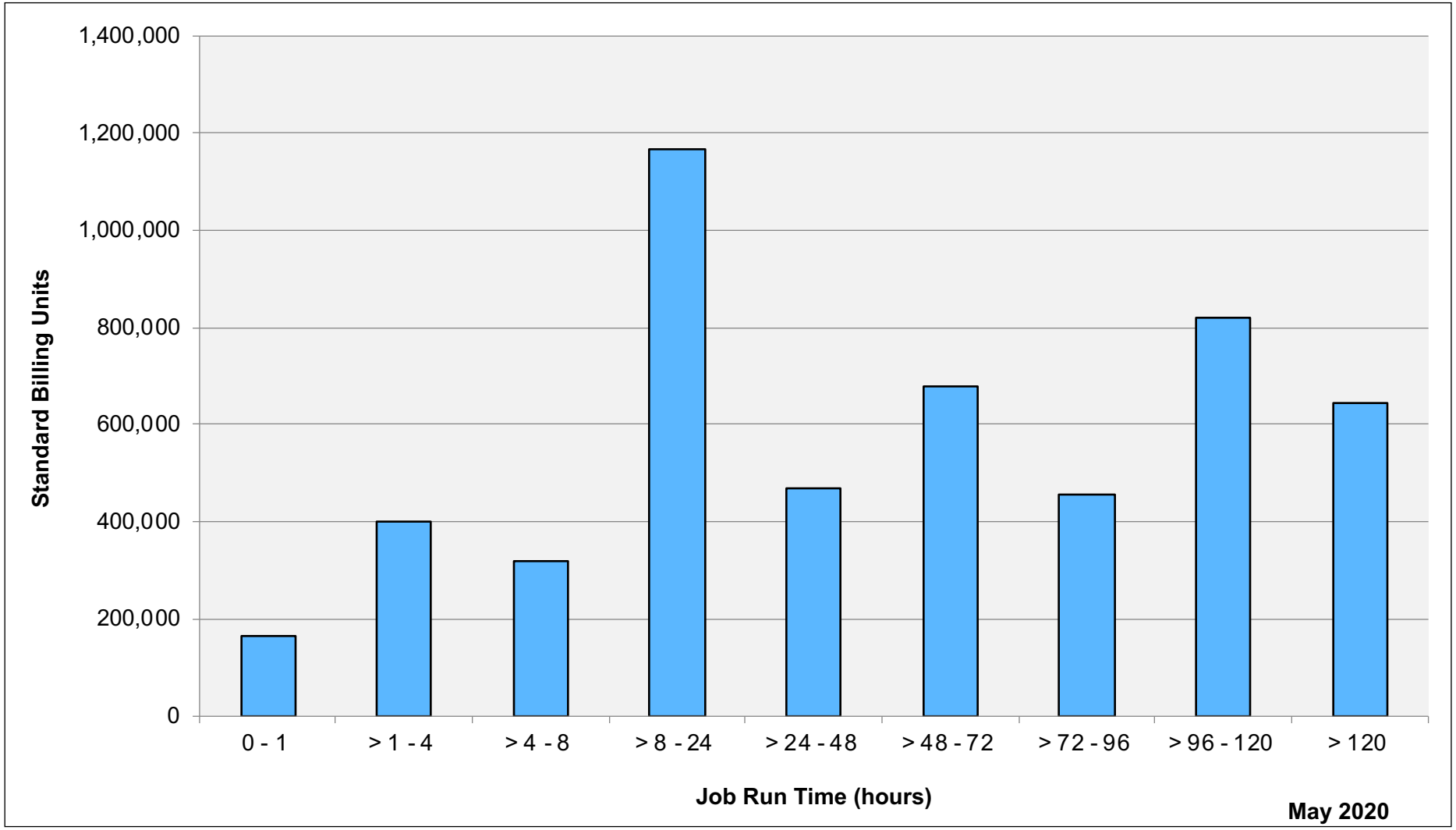
Pleiades: SBUs Reported, Normalized to 30-Day Month



Pleiades: Devel Queue Utilization



Pleiades: Monthly Utilization by Job Length



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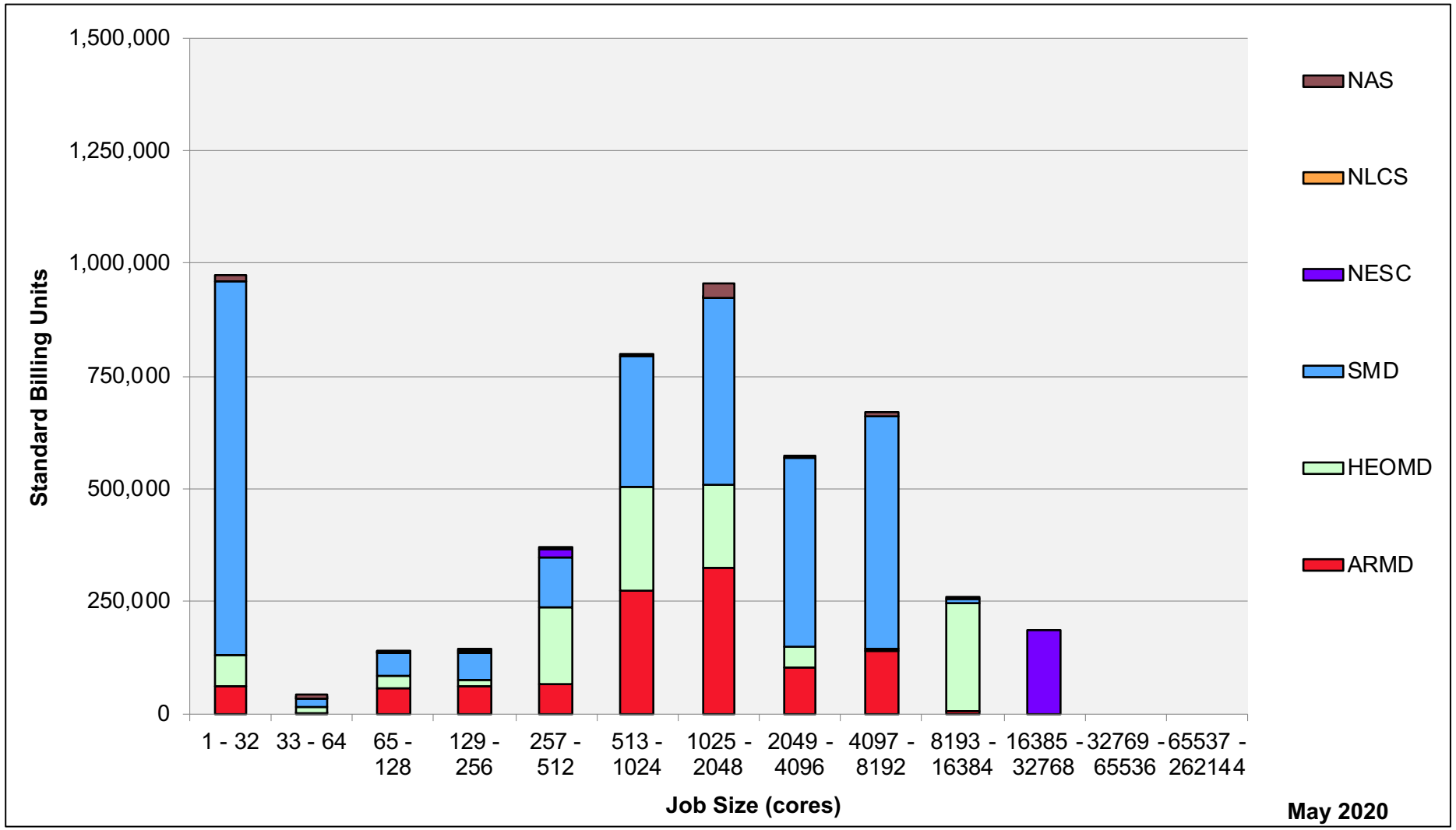
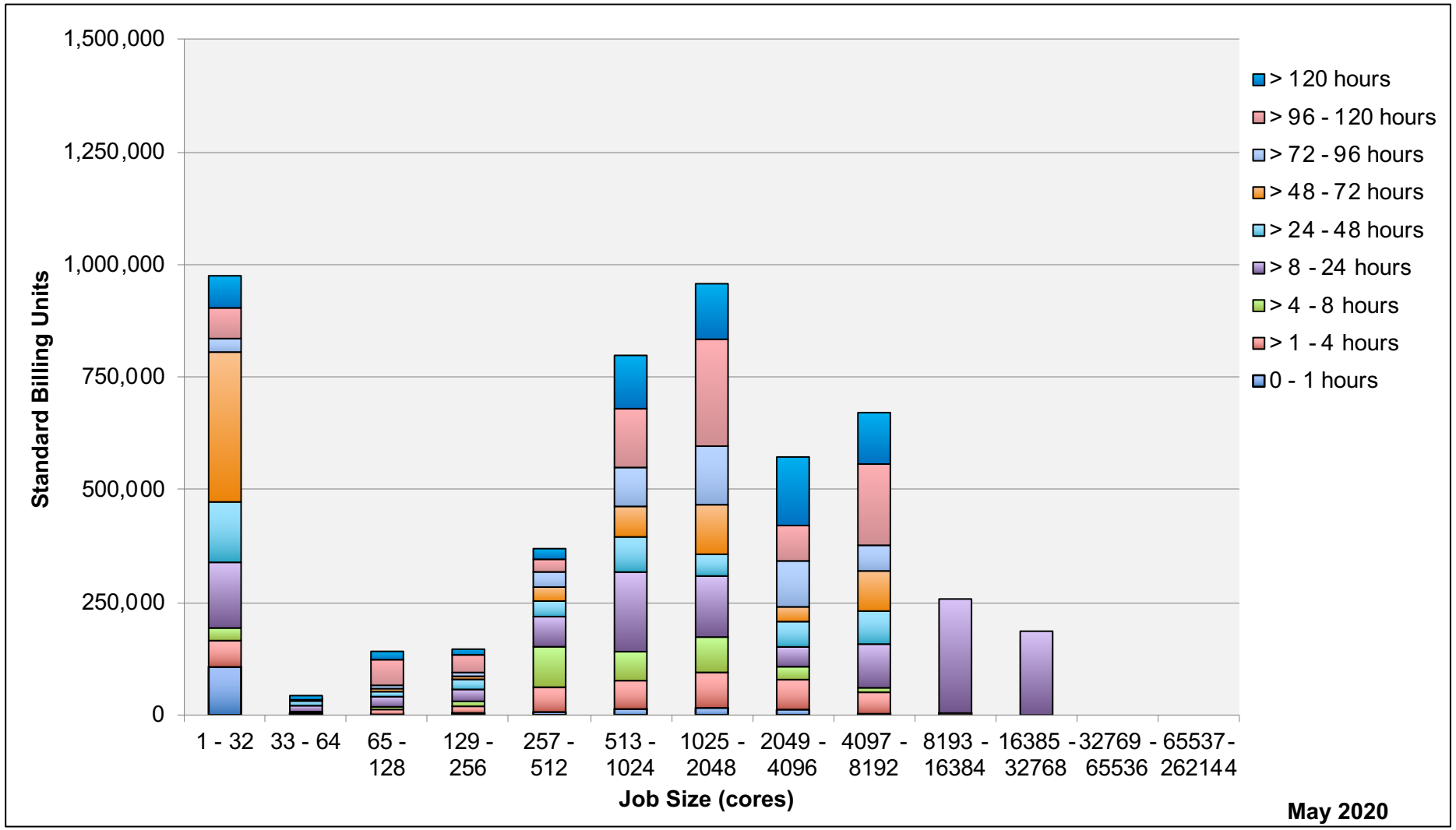
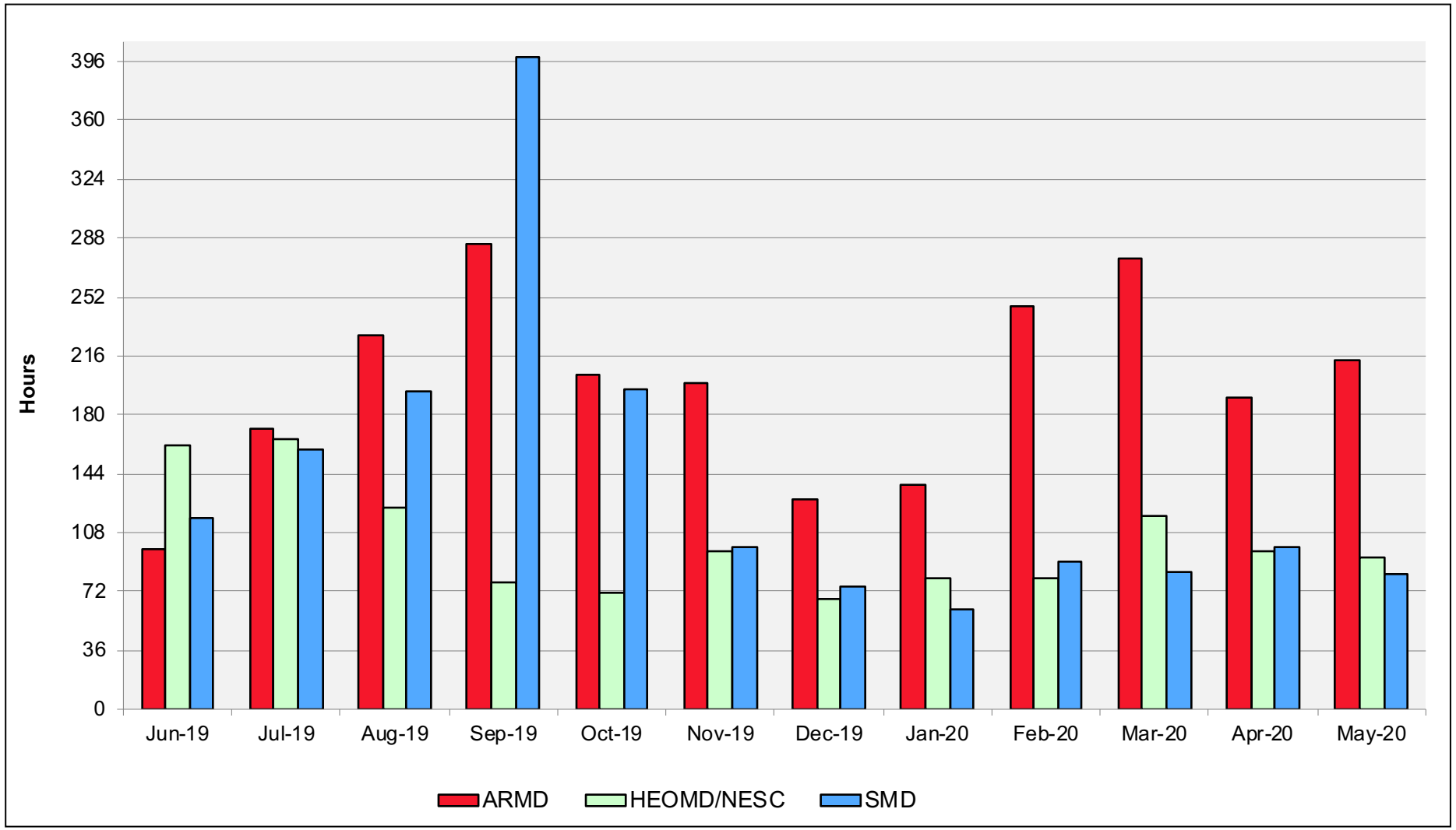


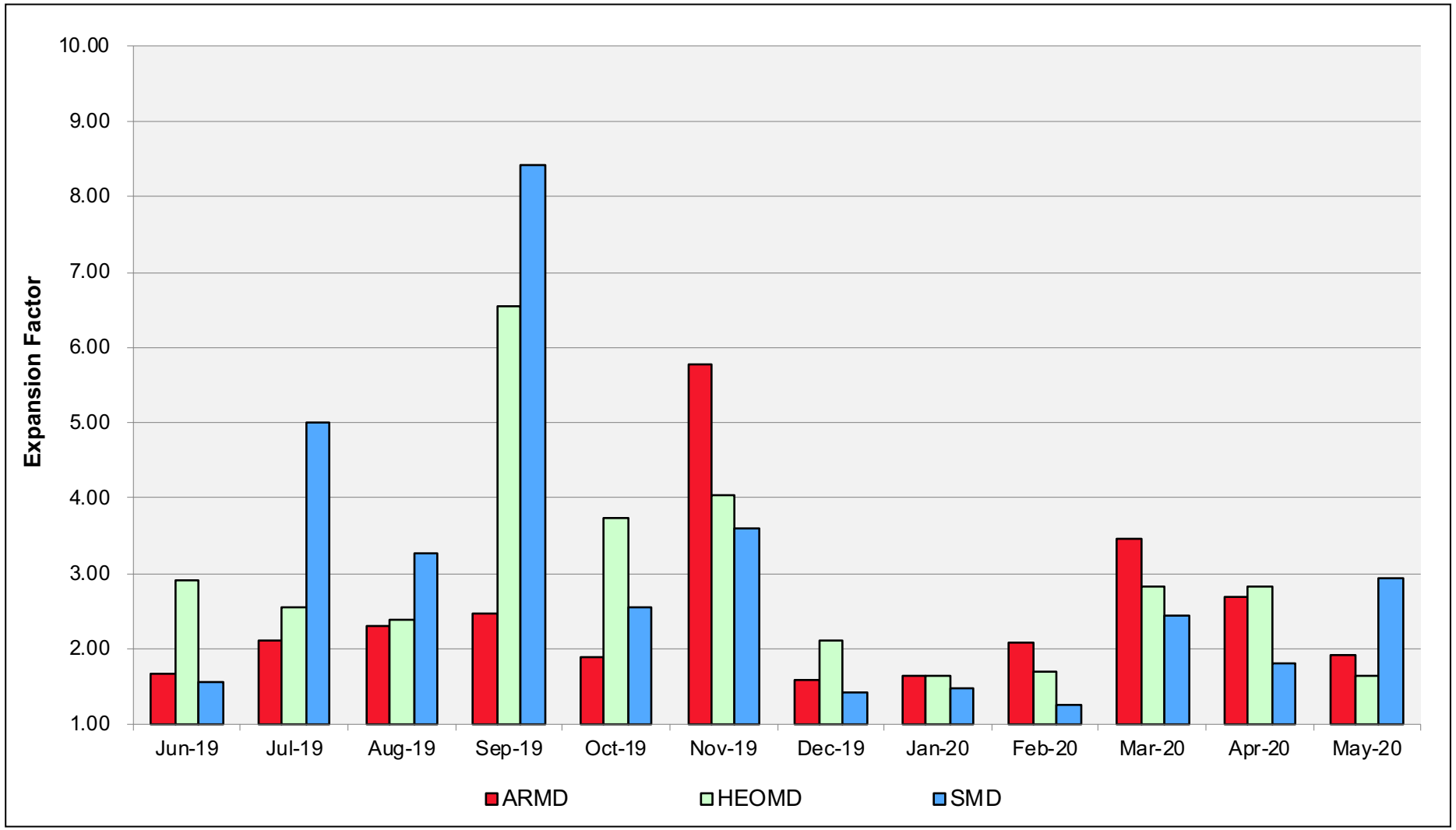
Pleiades: Monthly Utilization by Size and Length



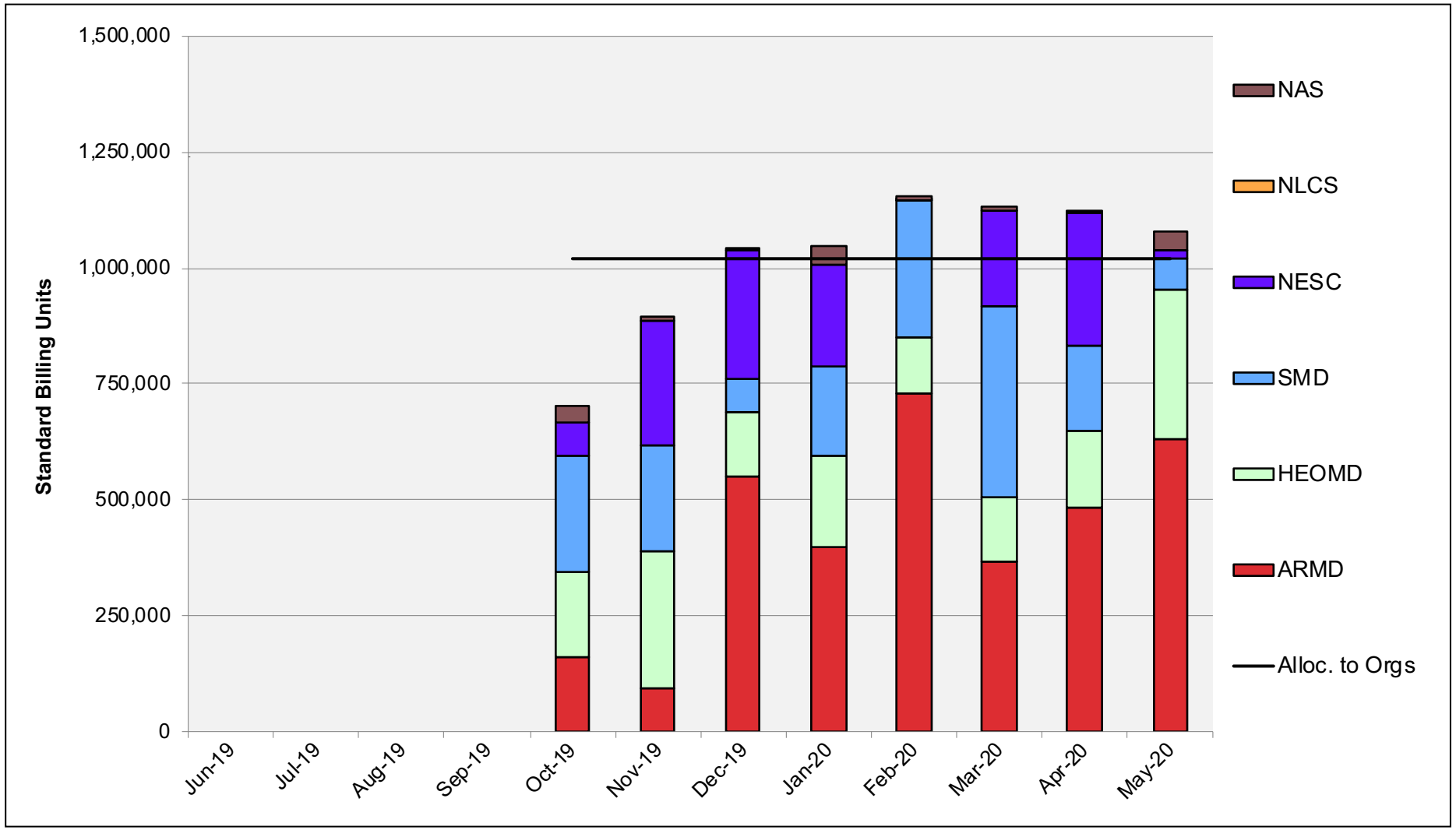
Pleiades: Average Time to Clear All Jobs



Pleiades: Average Expansion Factor



Aitken: SBUs Reported, Normalized to 30-Day Month



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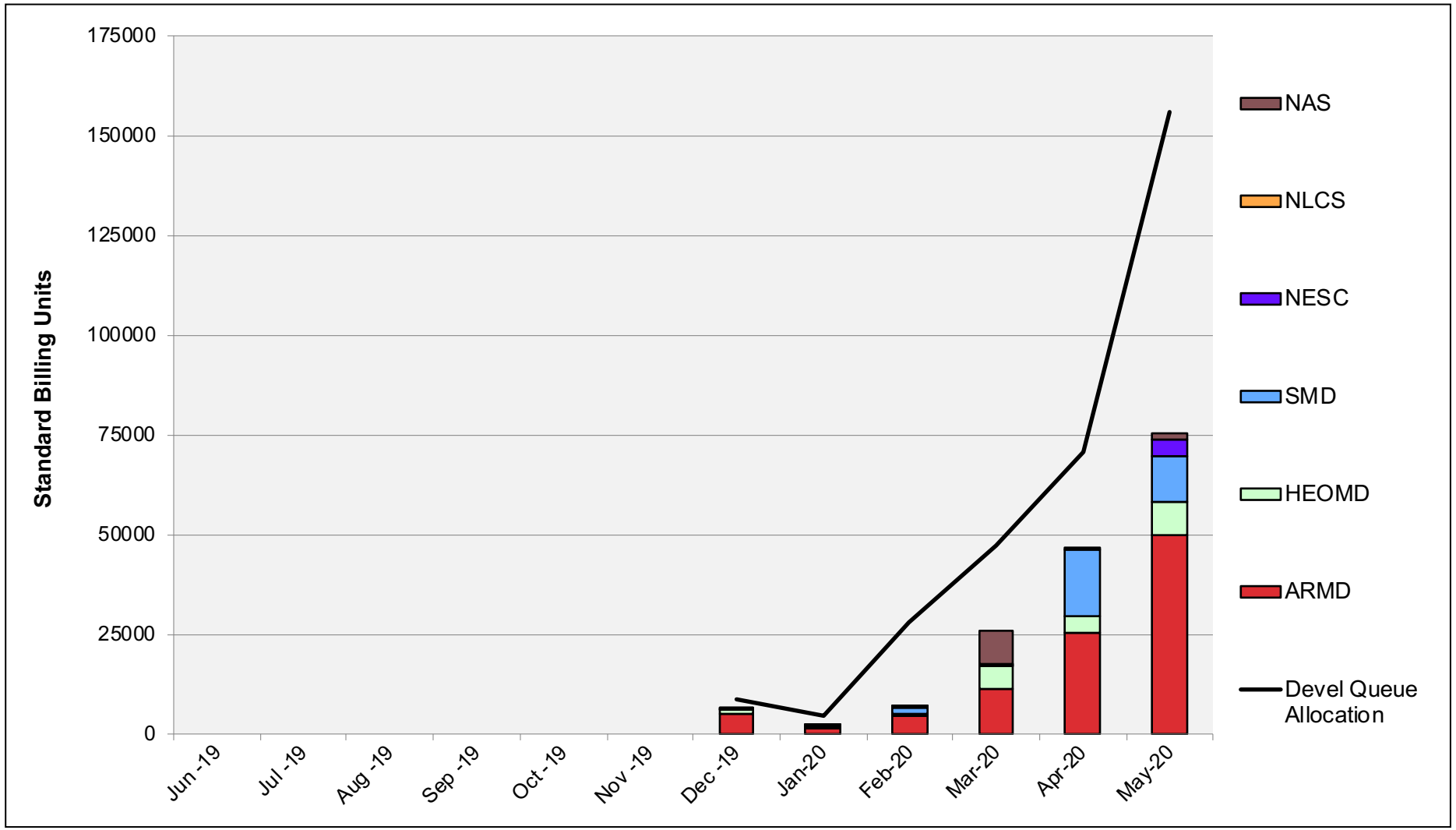

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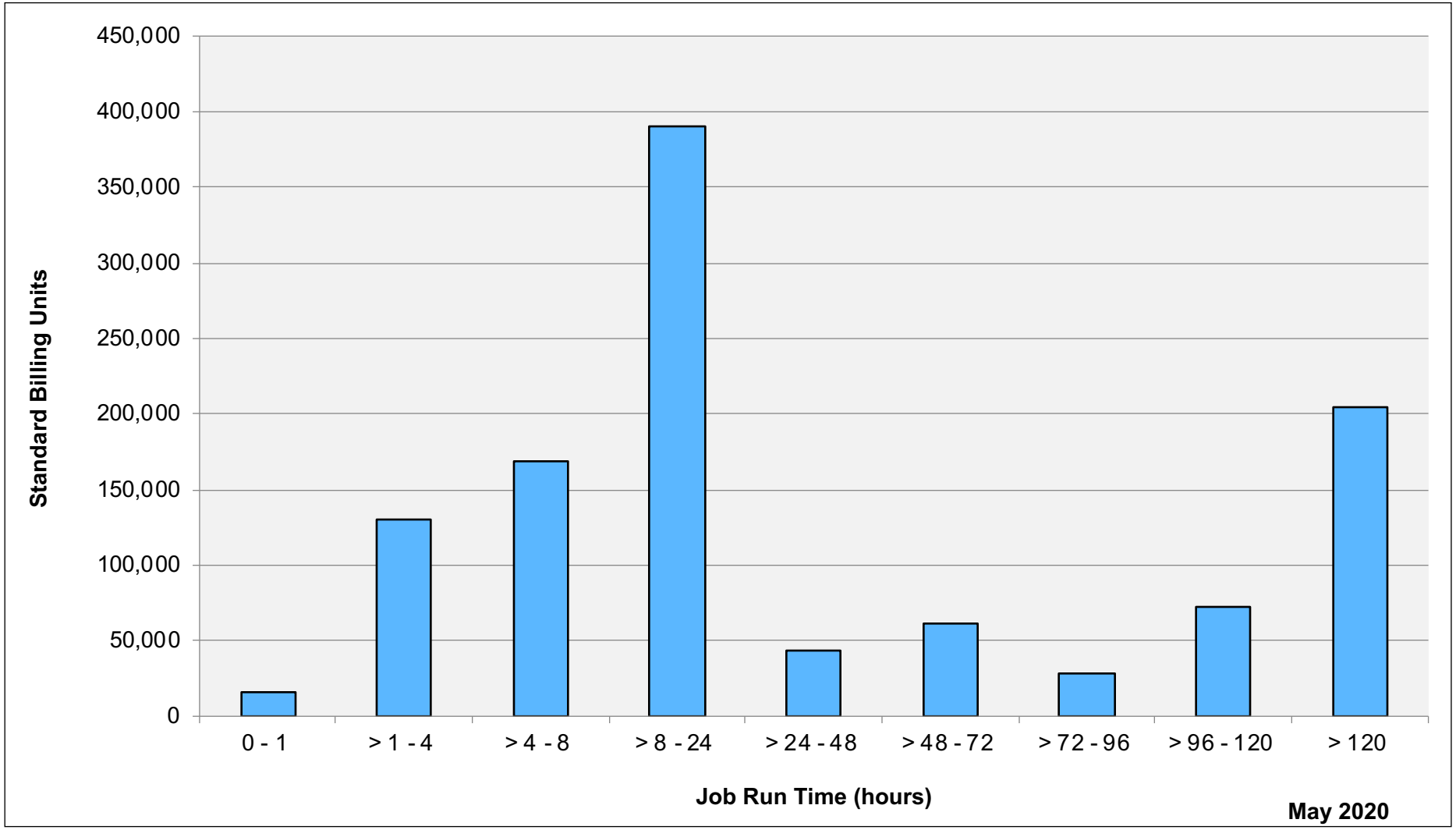

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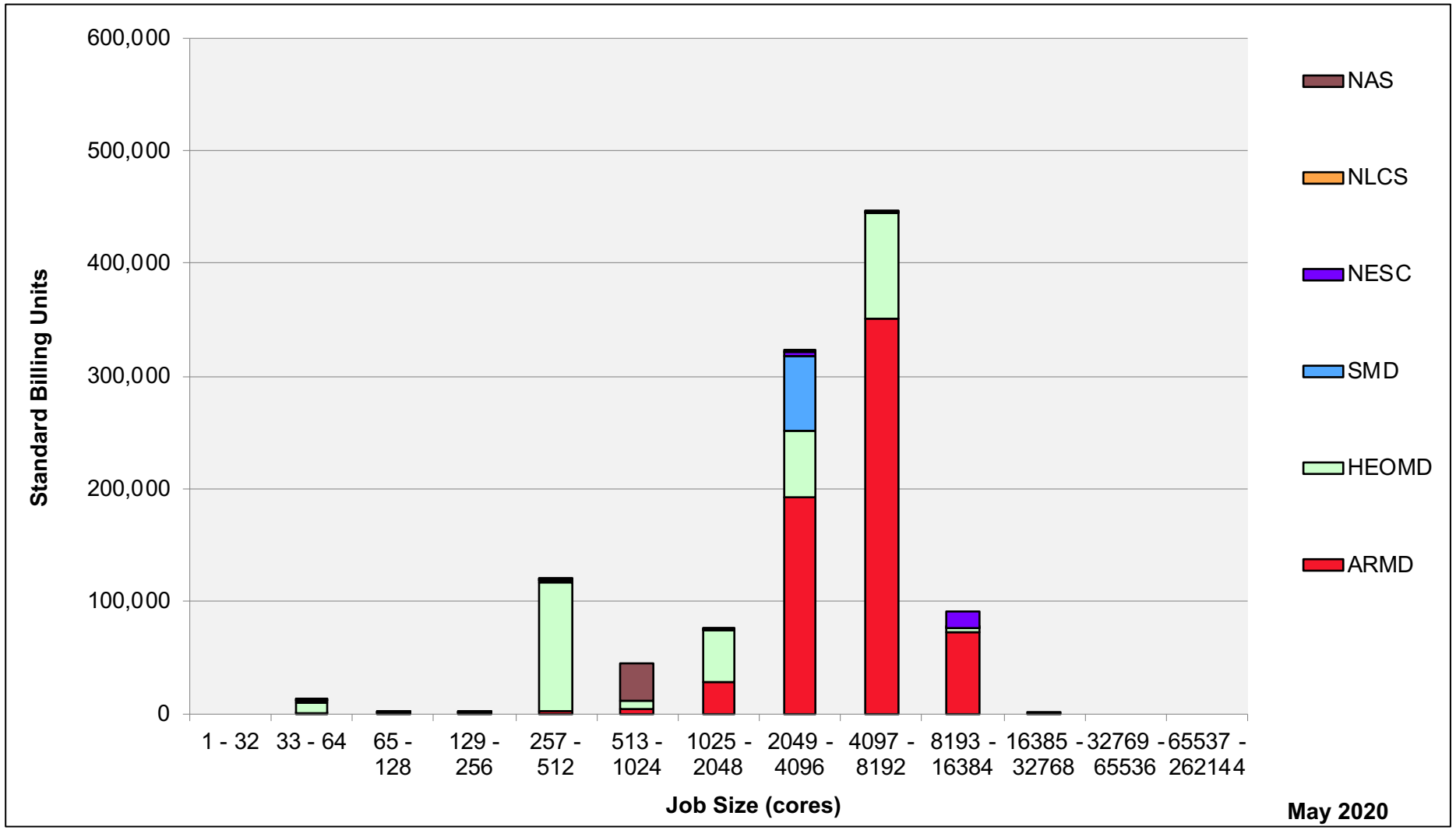

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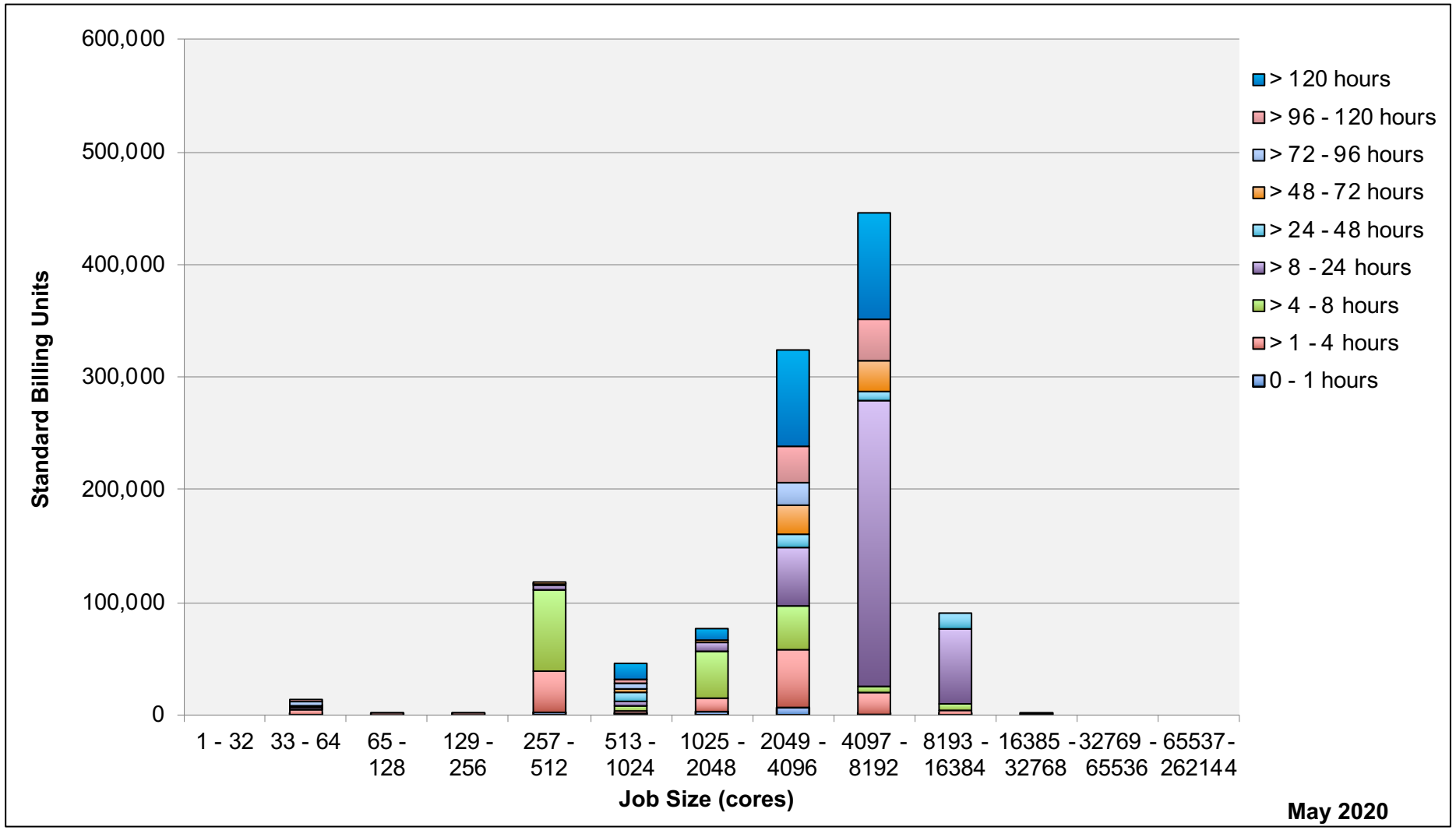

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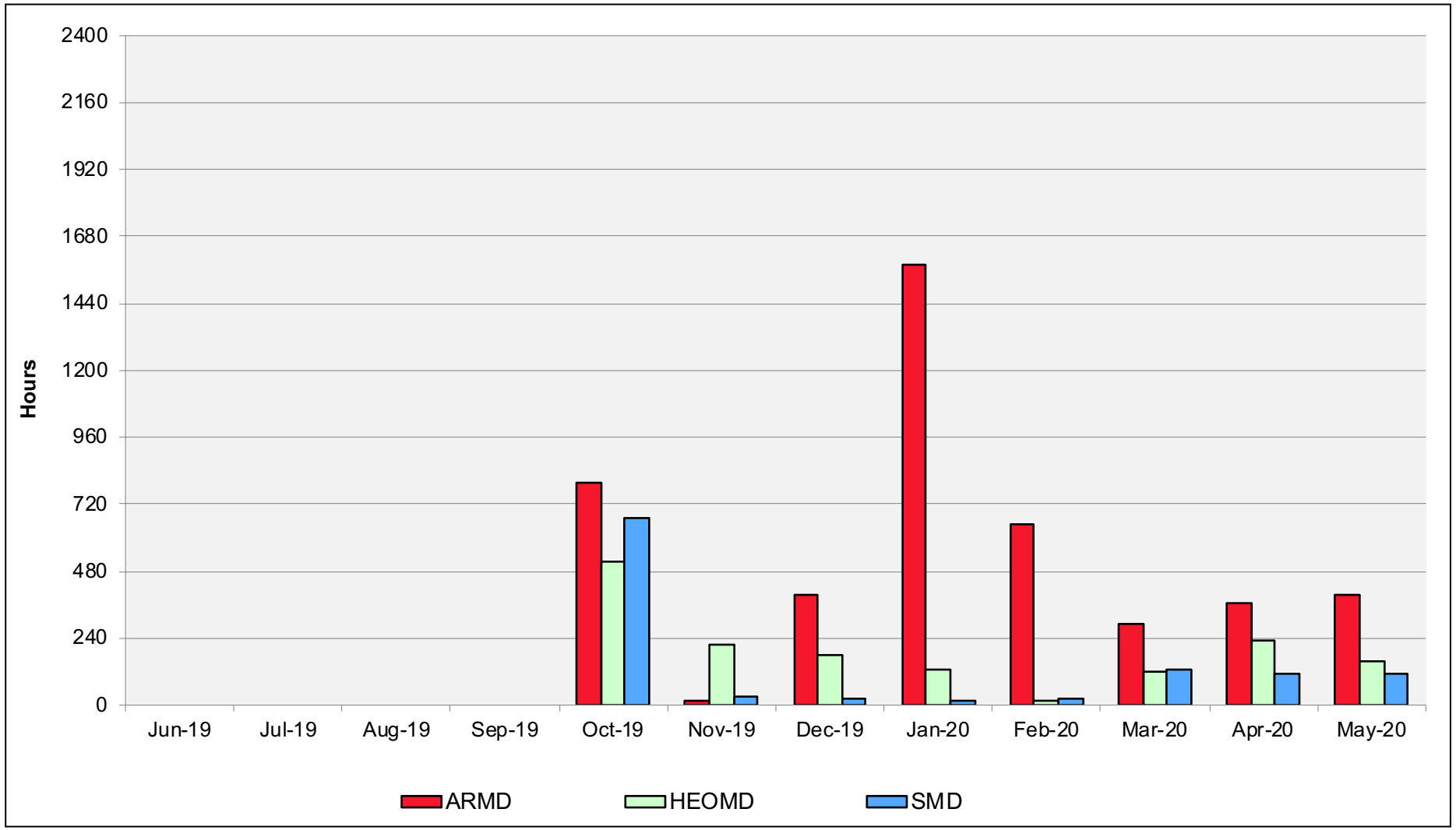

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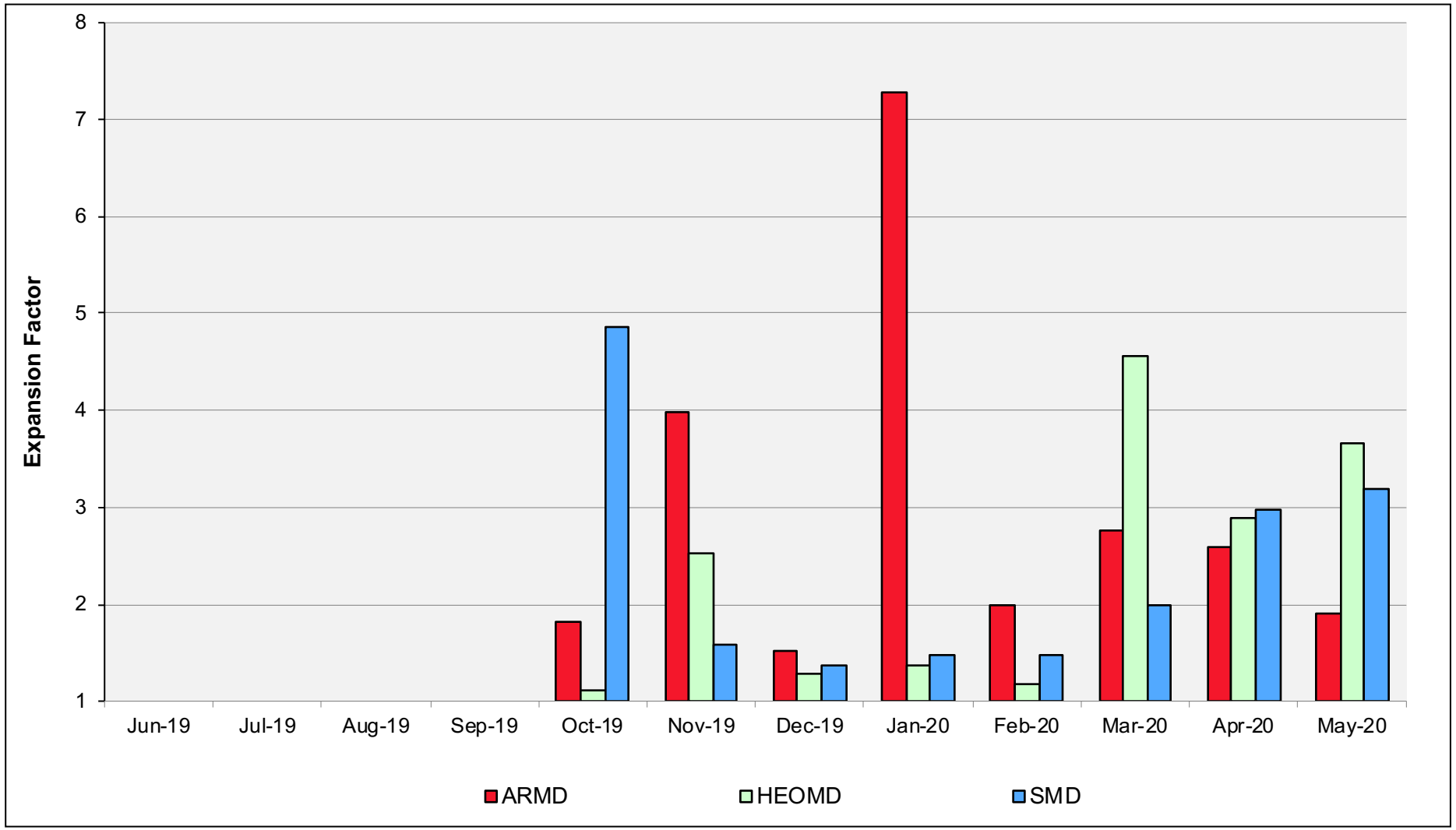

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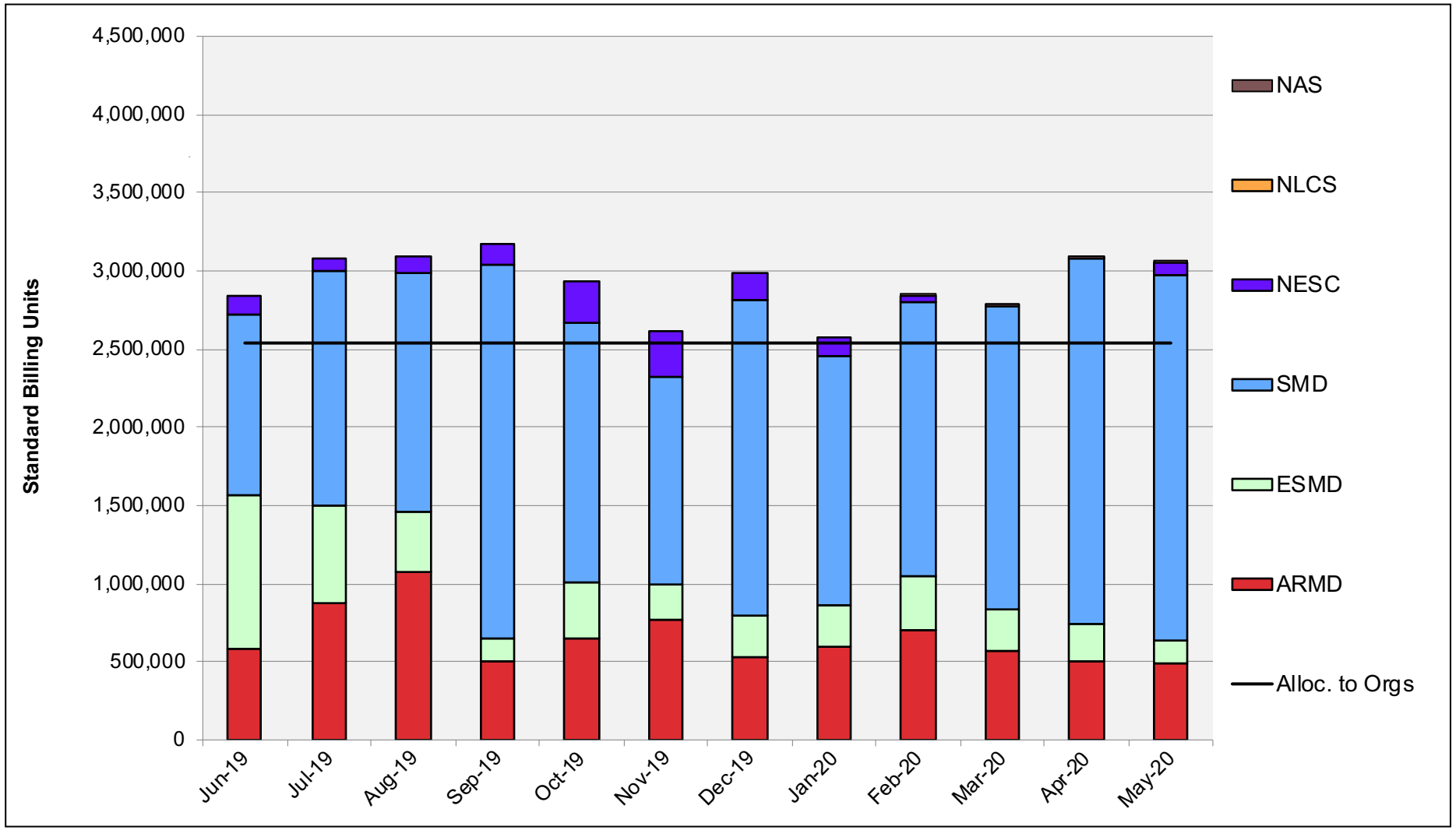

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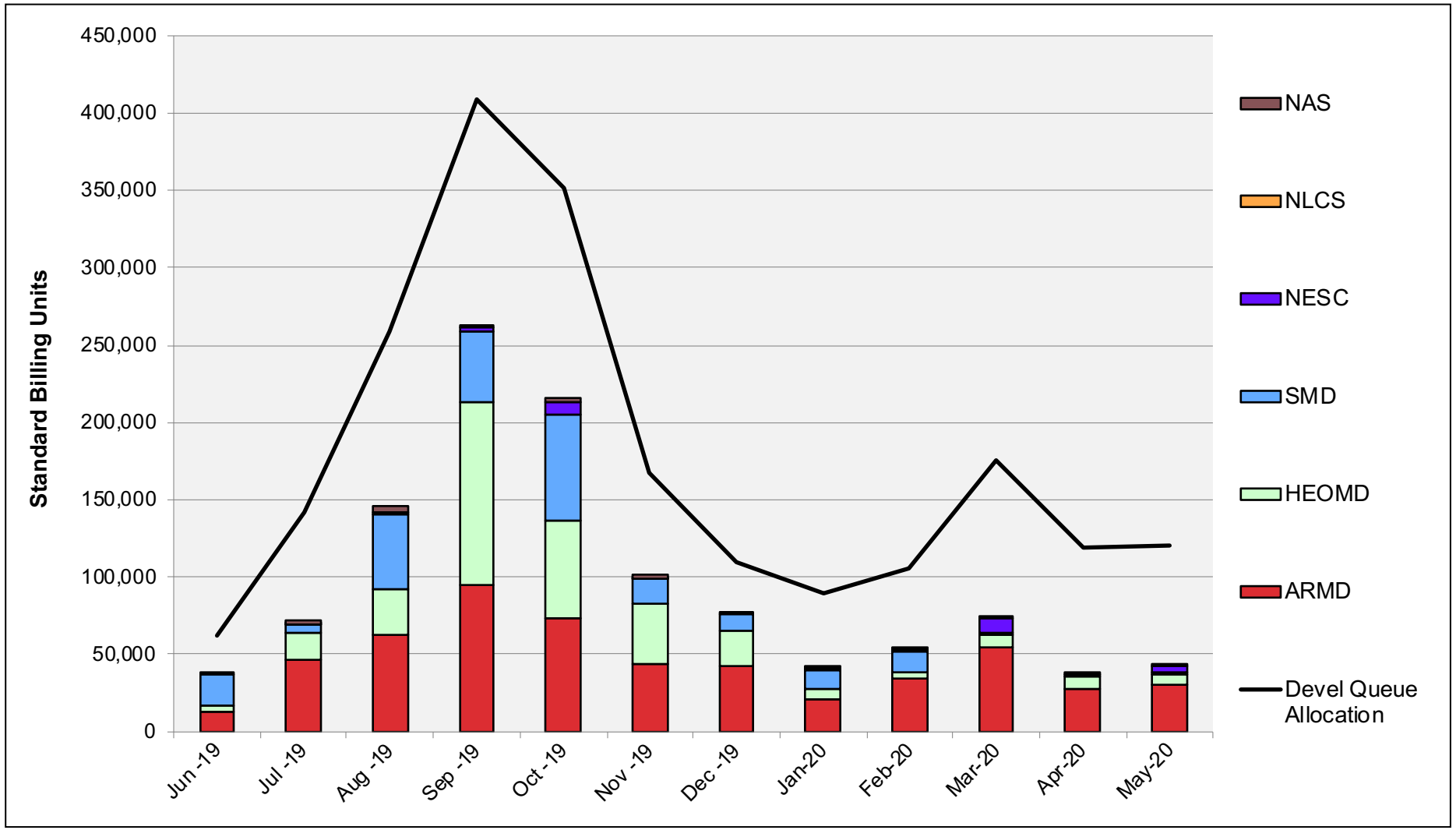

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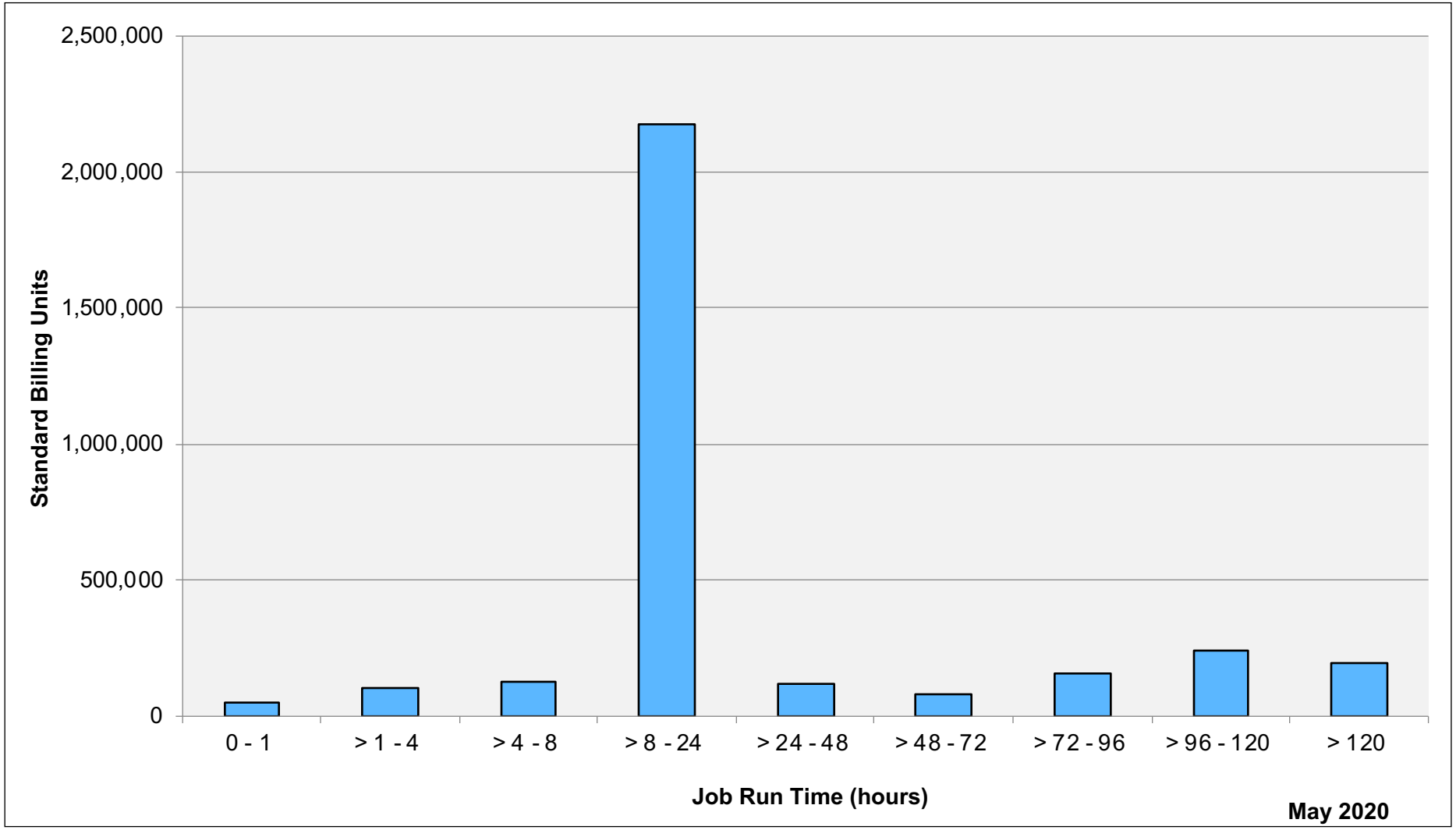
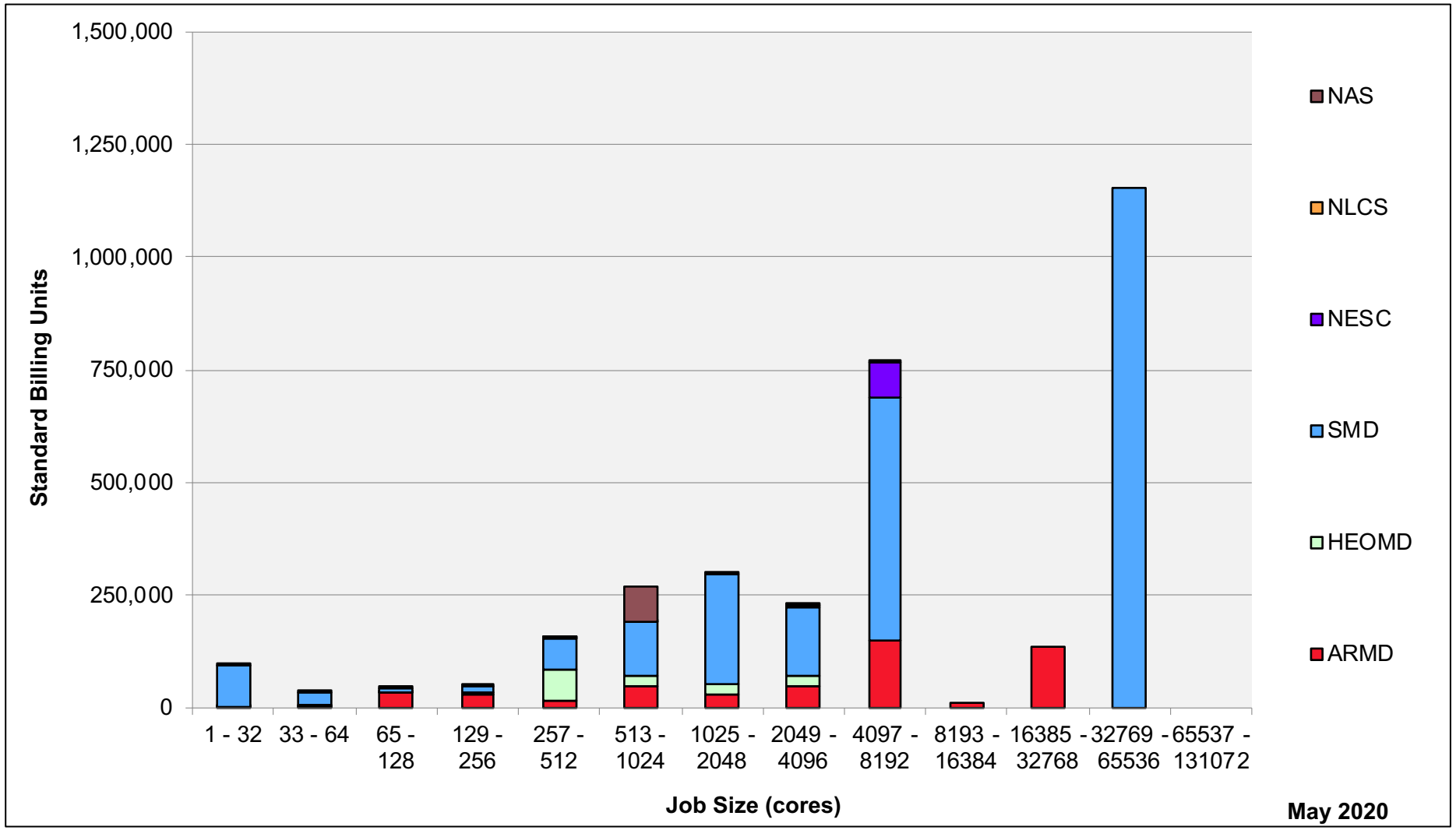
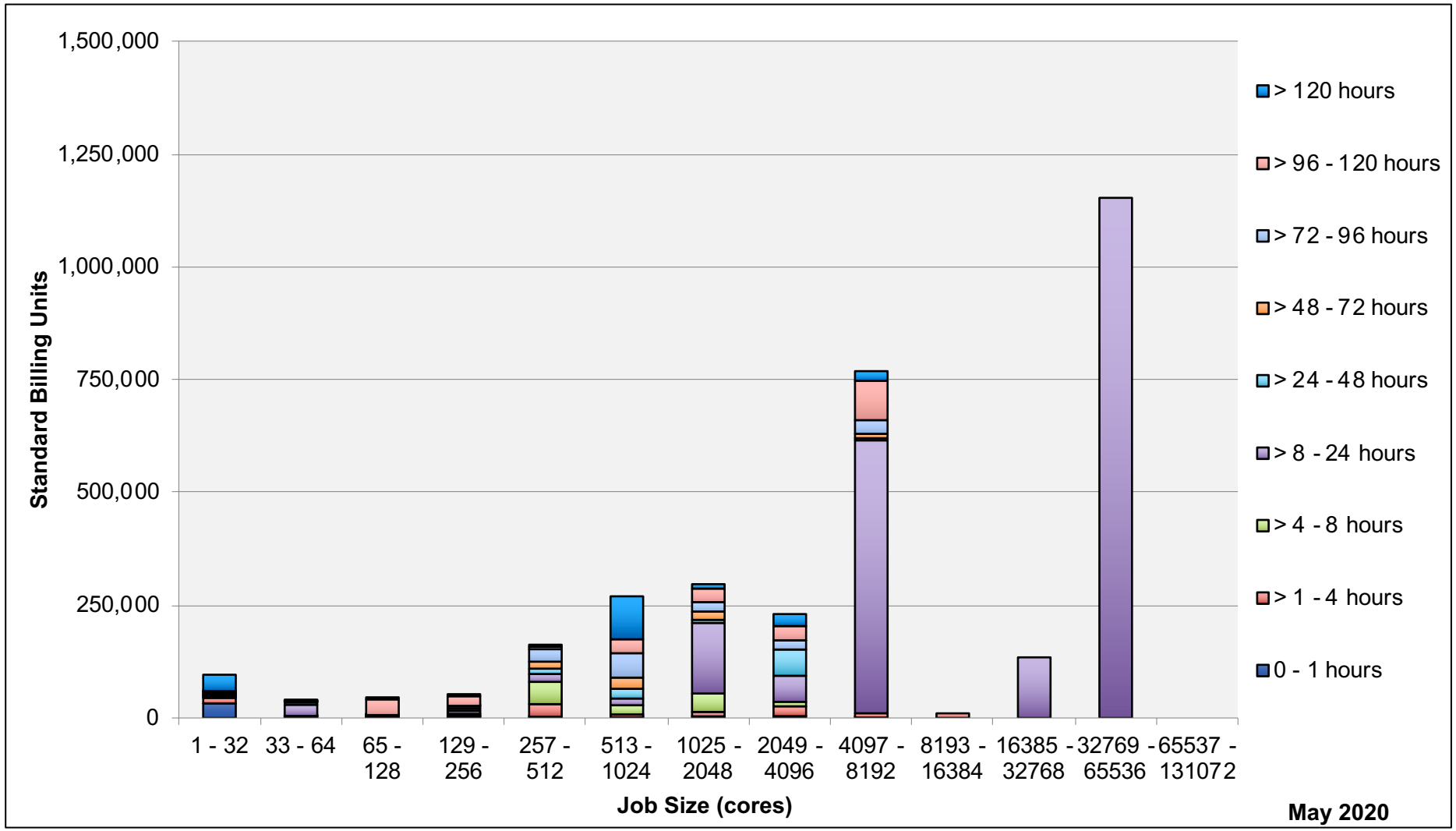


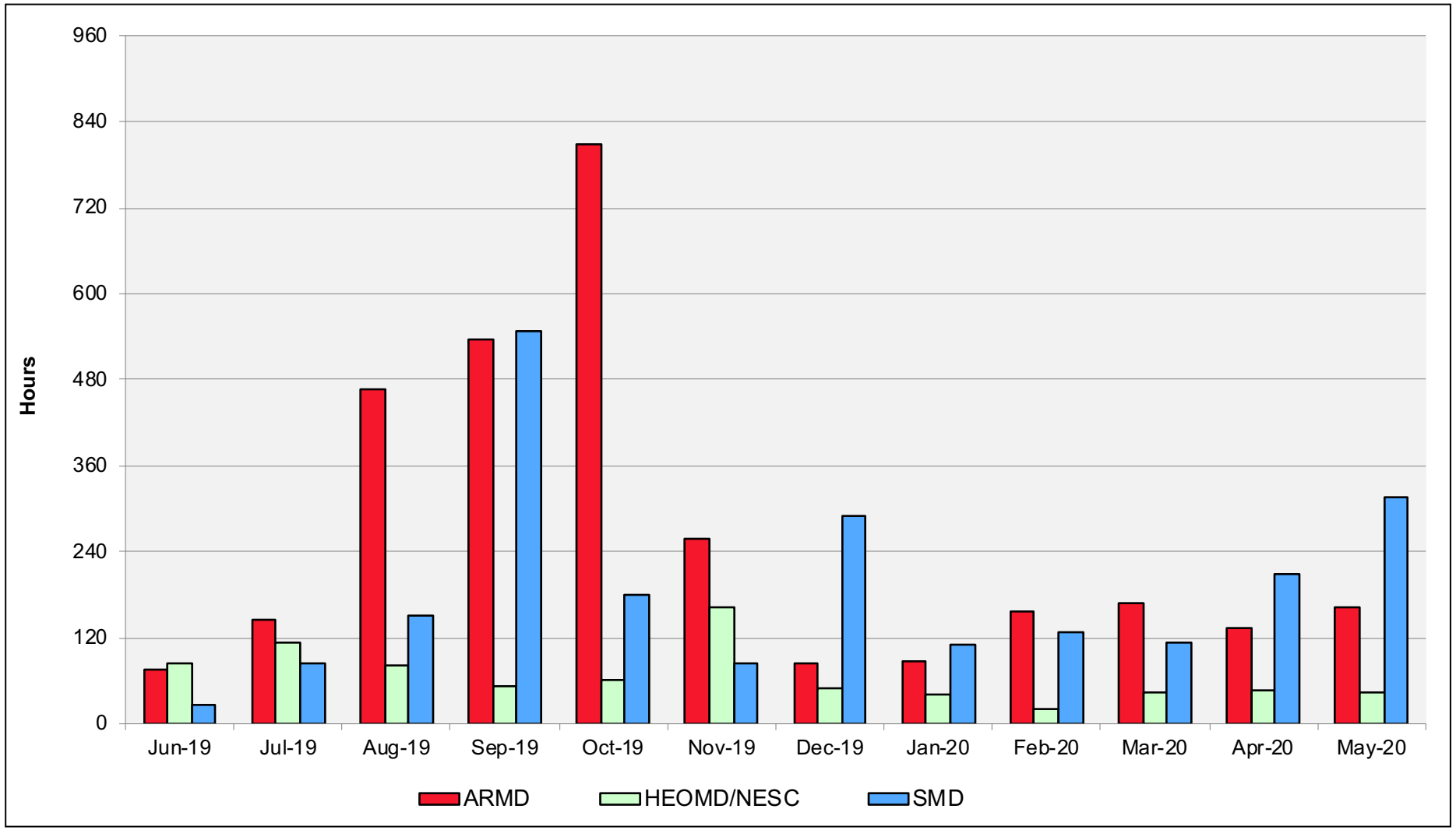
Electra: Monthly Utilization by Job Length



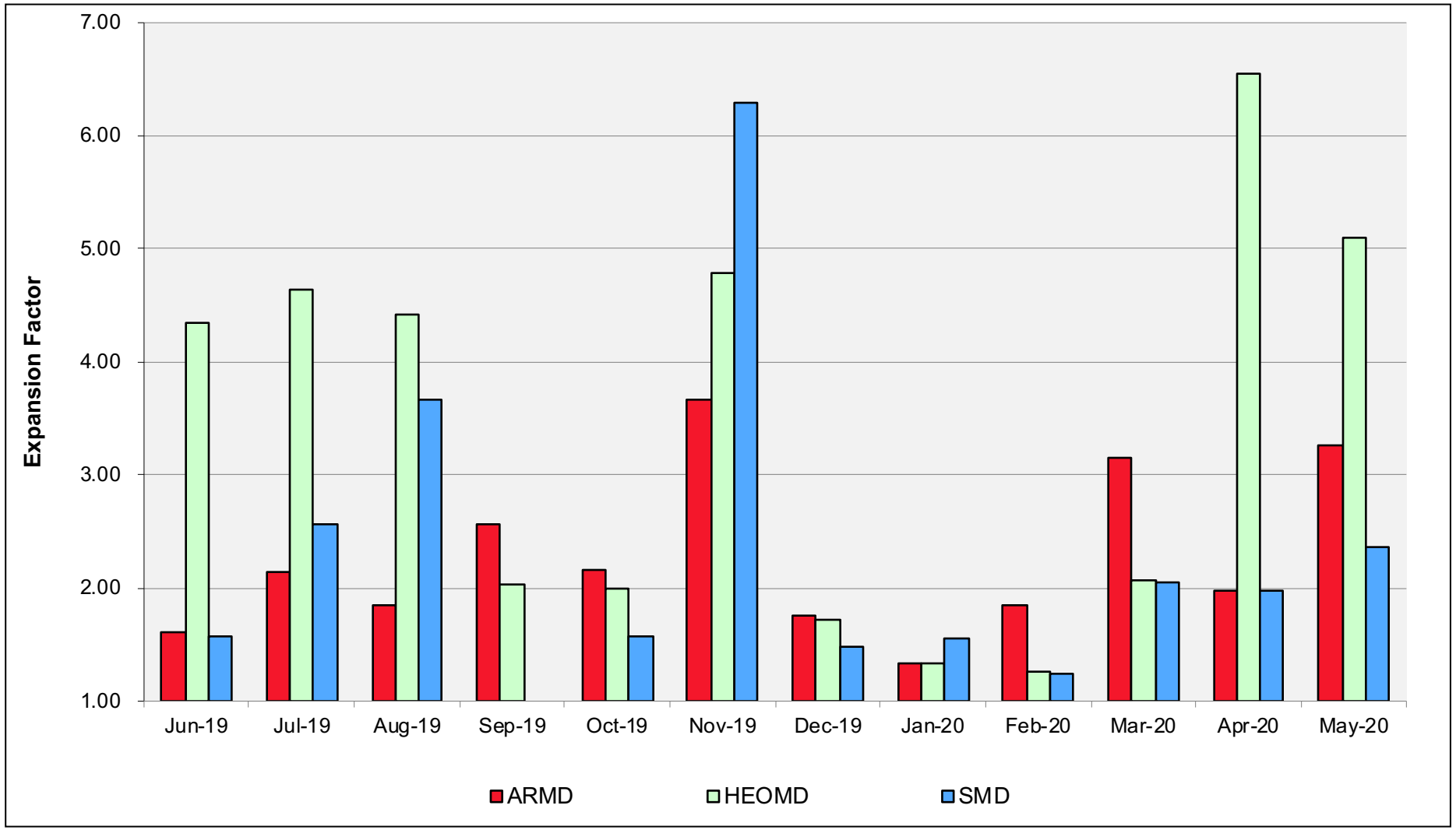
Electra: Monthly Utilization by Size and Length



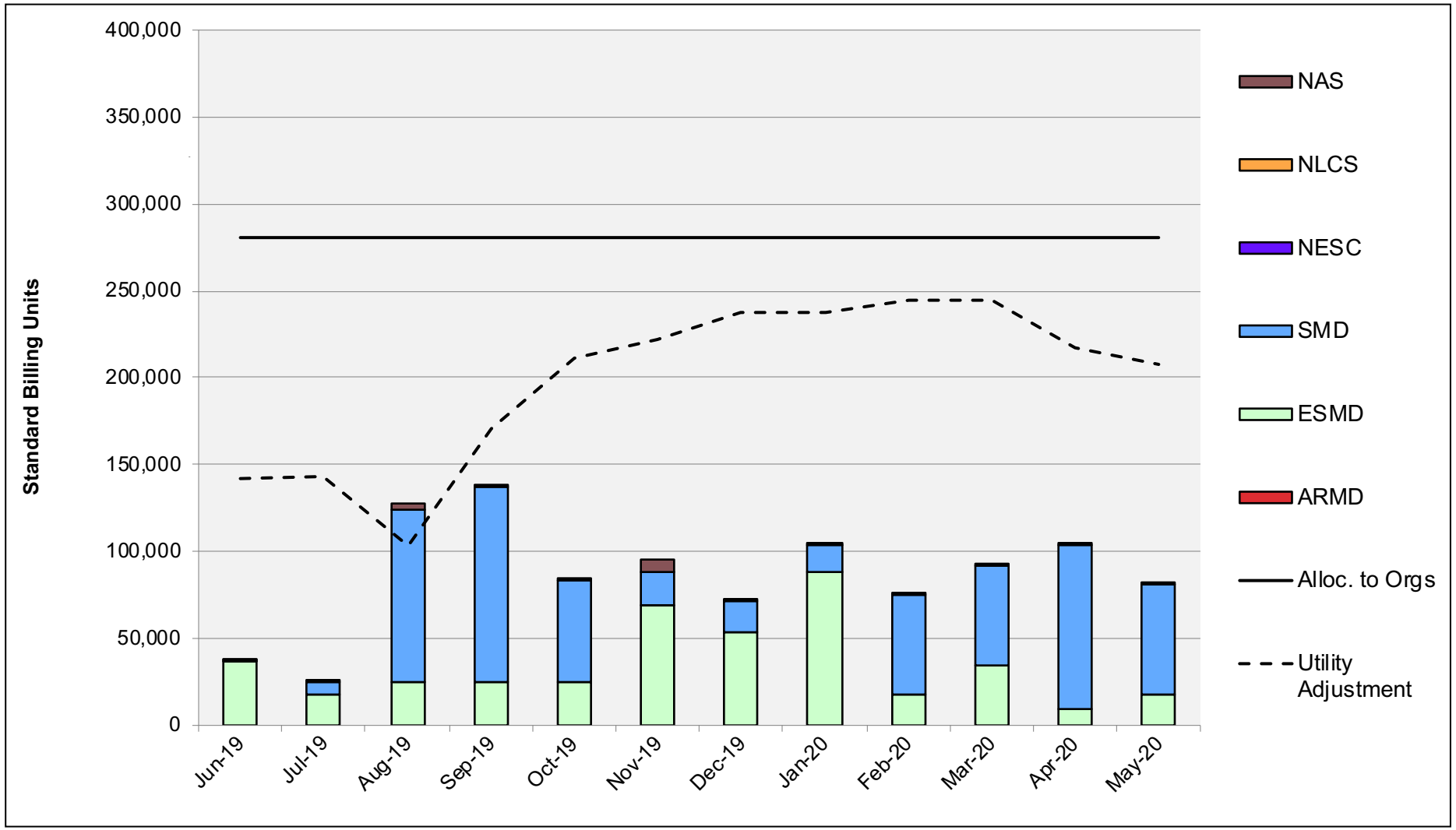
Electra: Average Time to Clear All Jobs



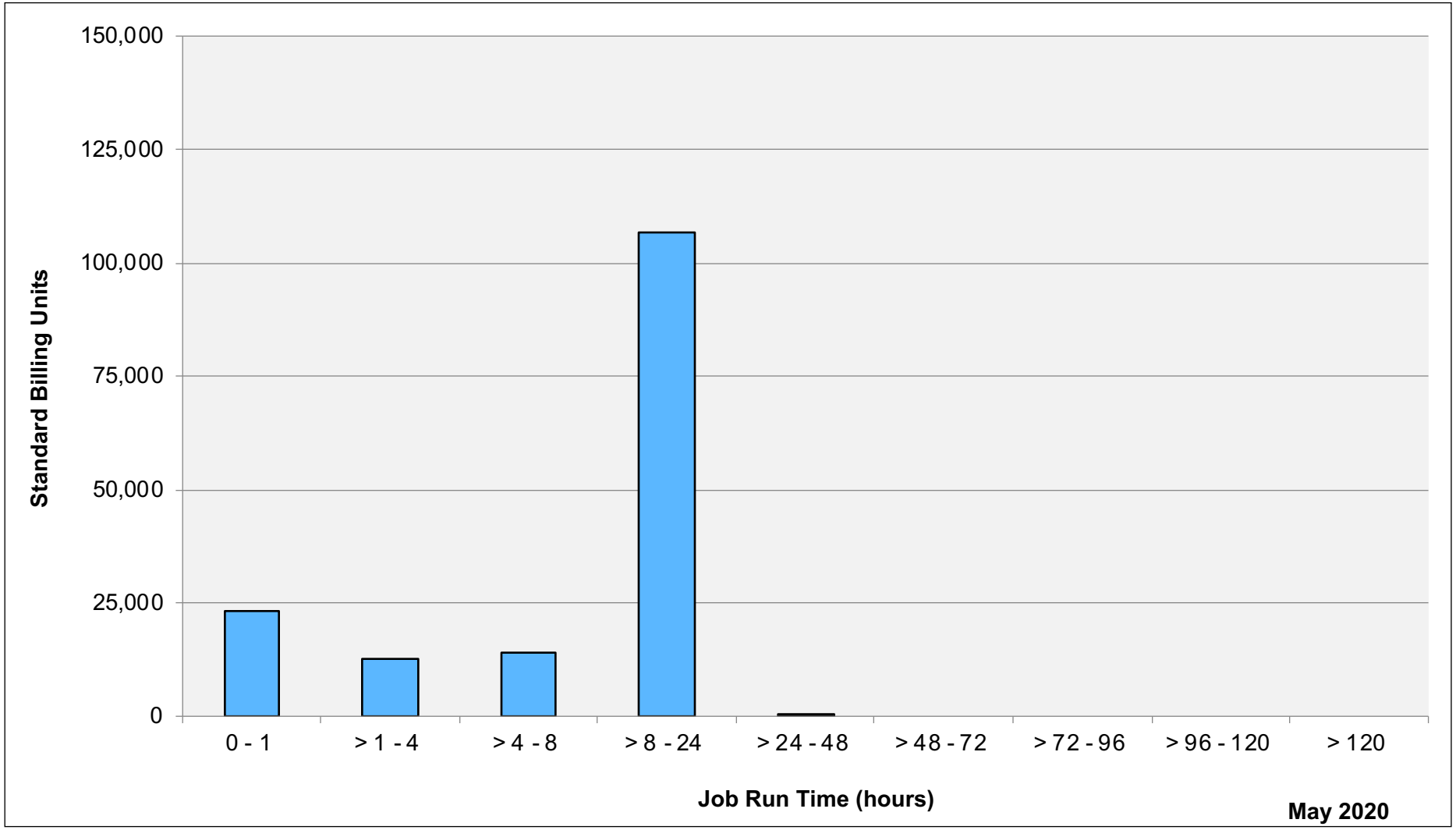
Electra: Average Expansion Factor



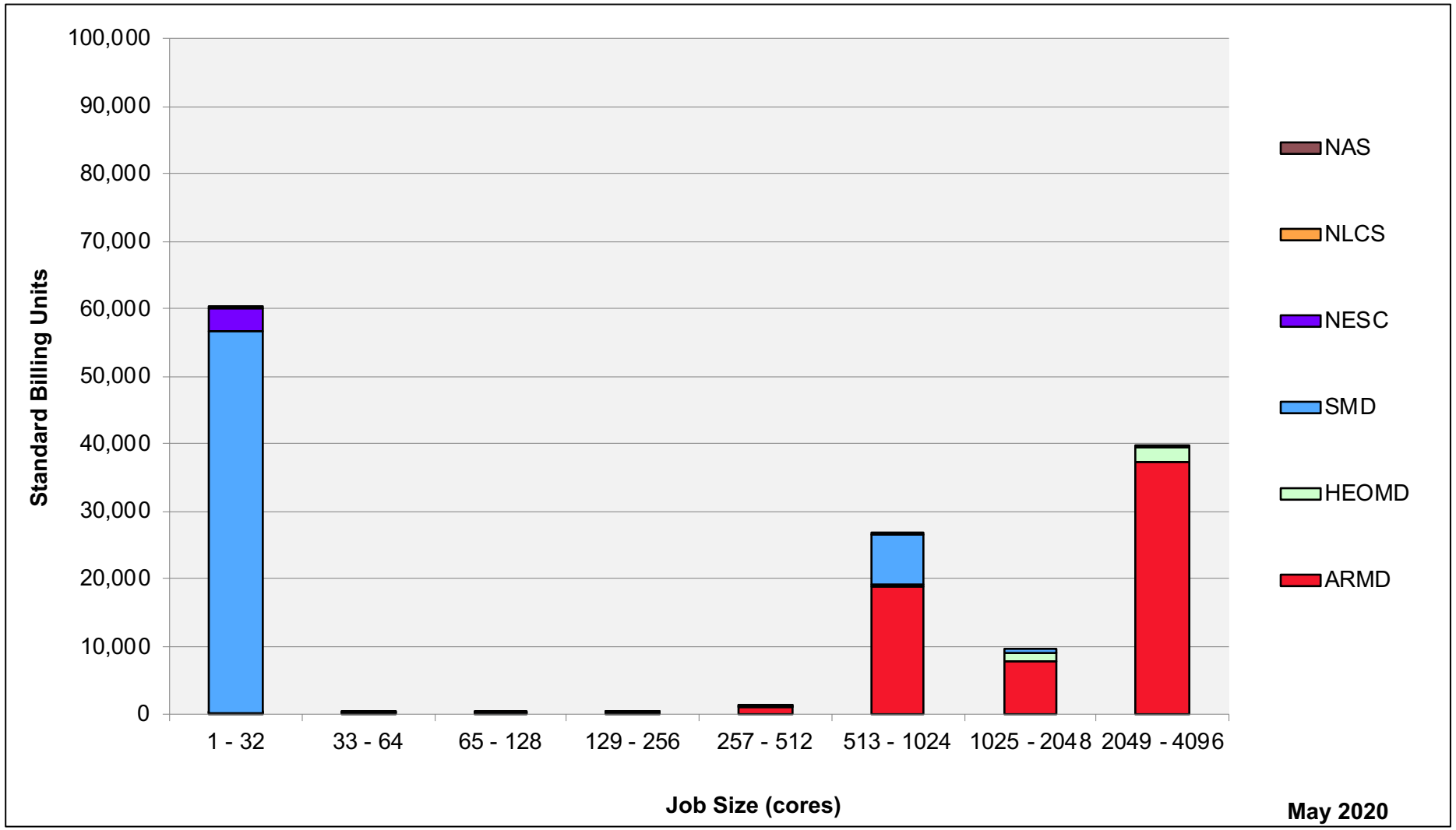
Merope: SBUs Reported, Normalized to 30-Day Month



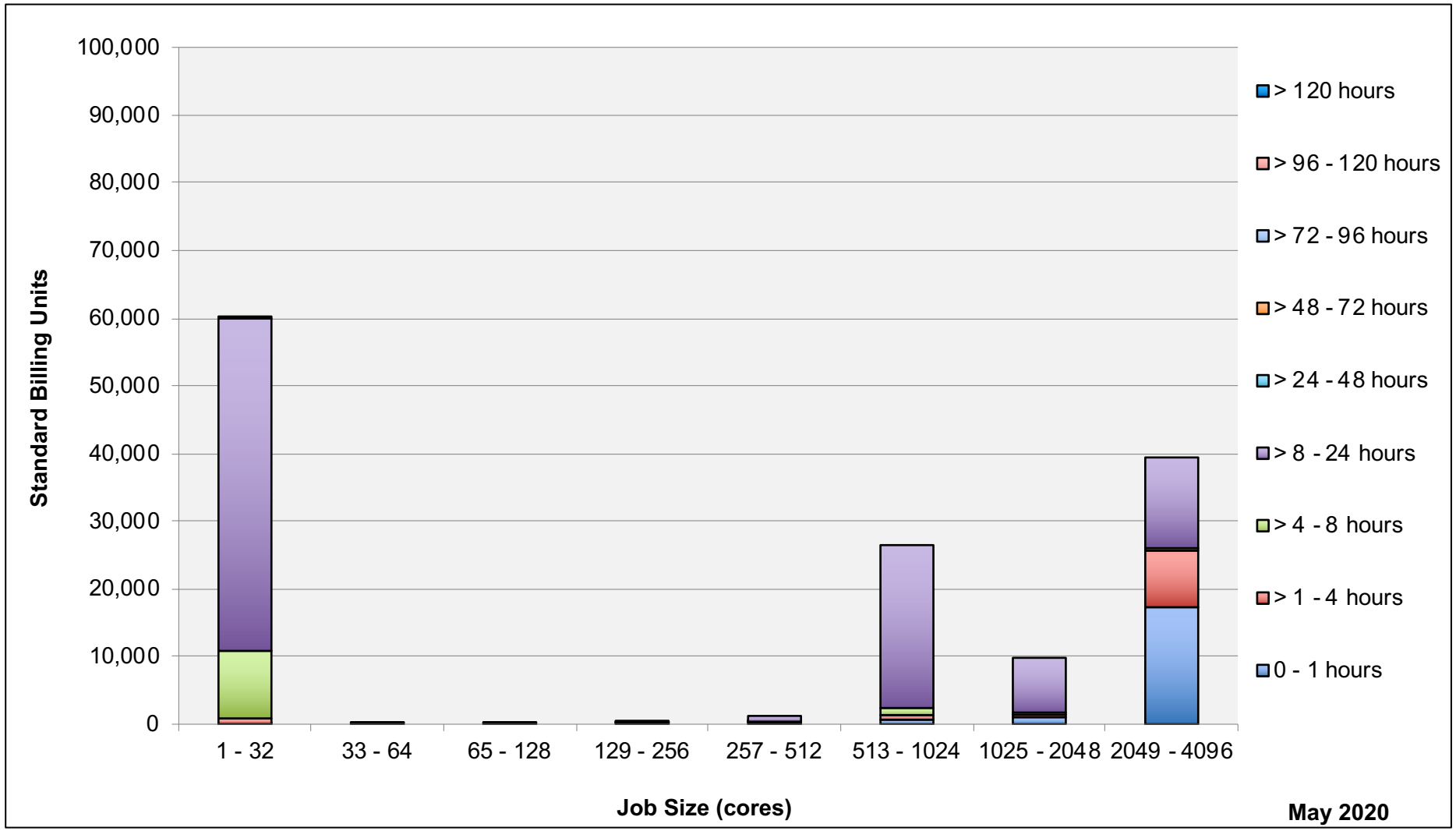
Merope: Monthly Utilization by Job Length



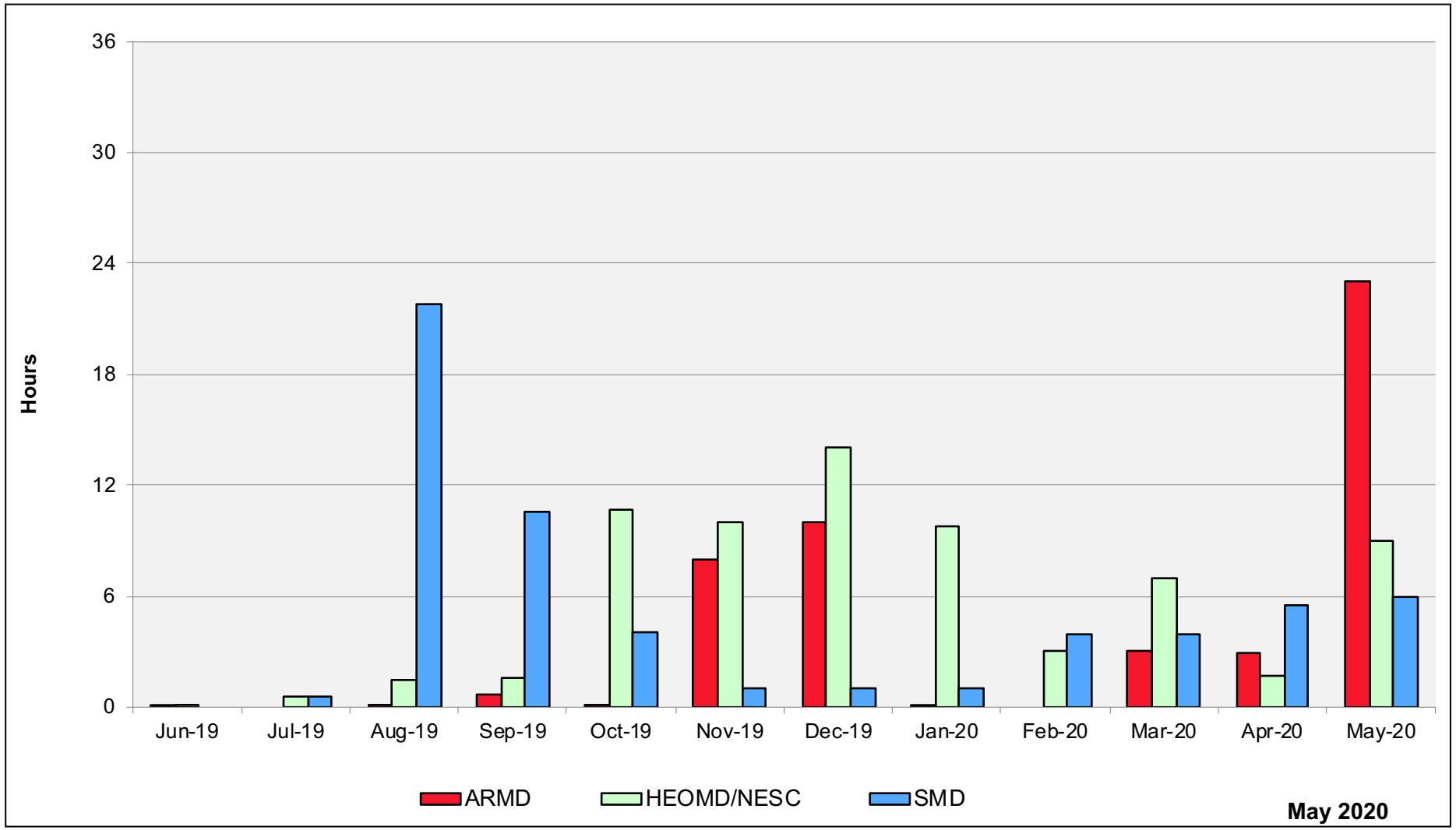
Merope: Monthly Utilization by Job Length



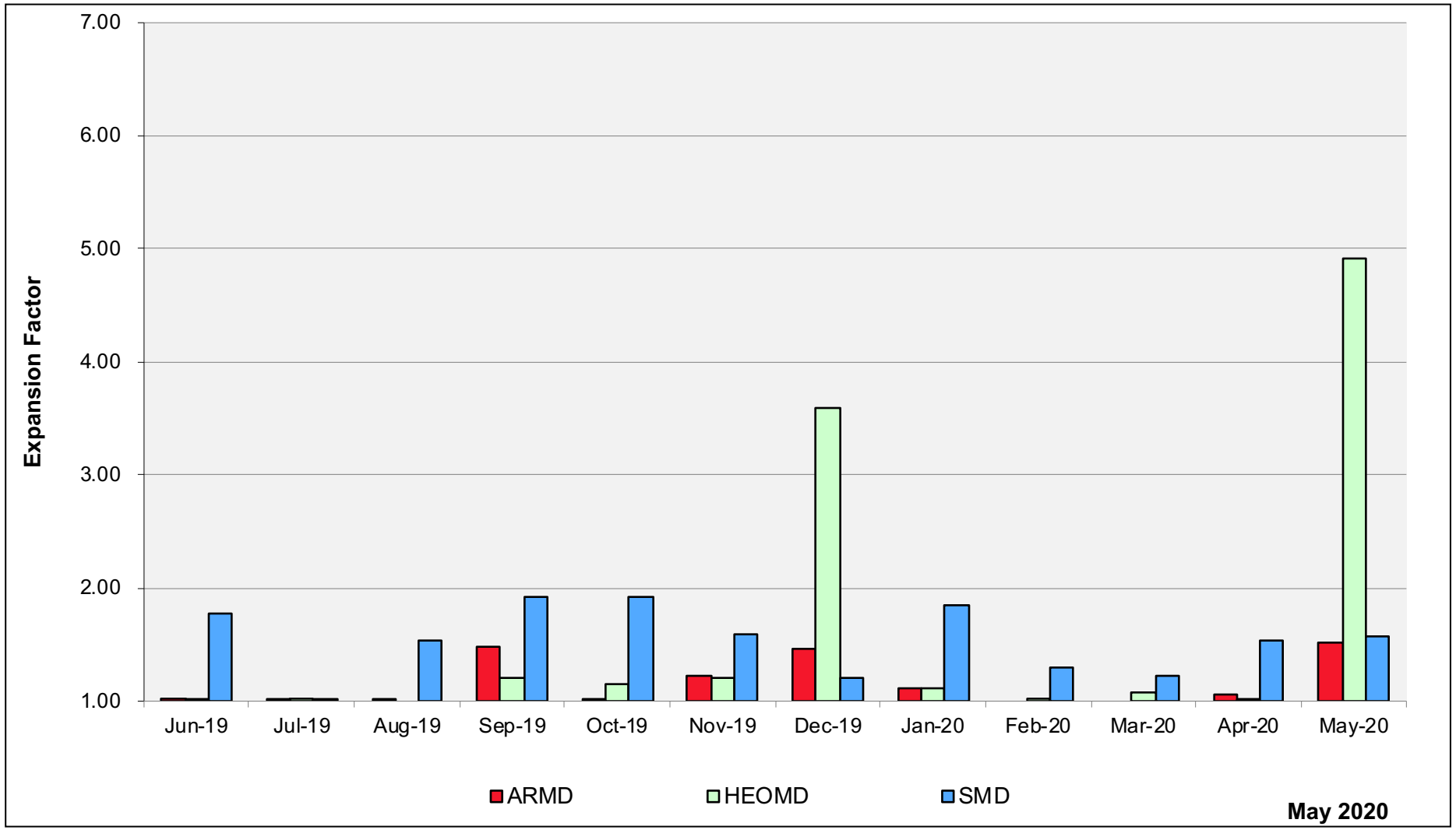
Merope: Monthly Utilization by Size and Length



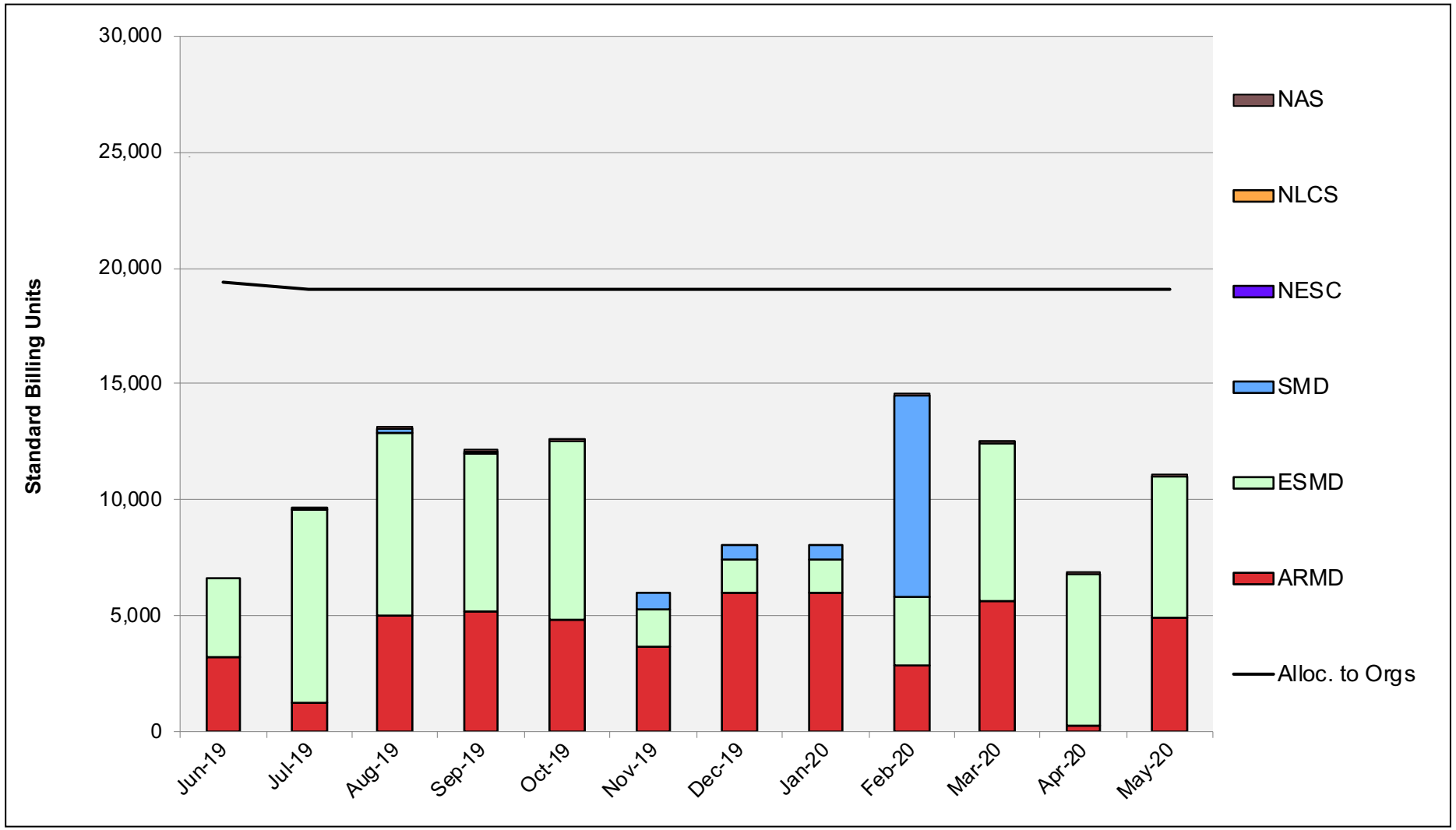
Merope: Average Time to Clear All Jobs



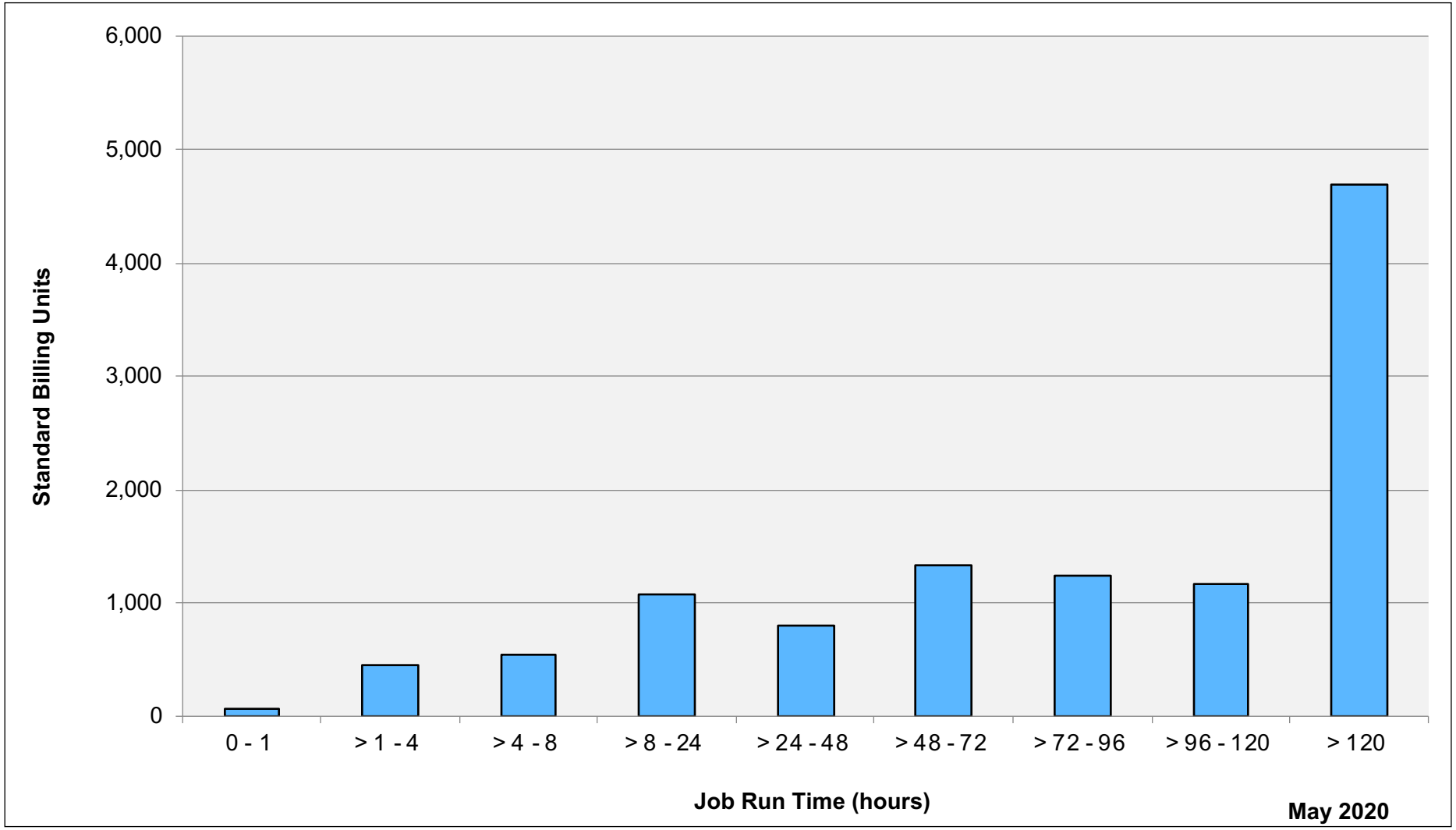
Merope: Average Expansion Factor



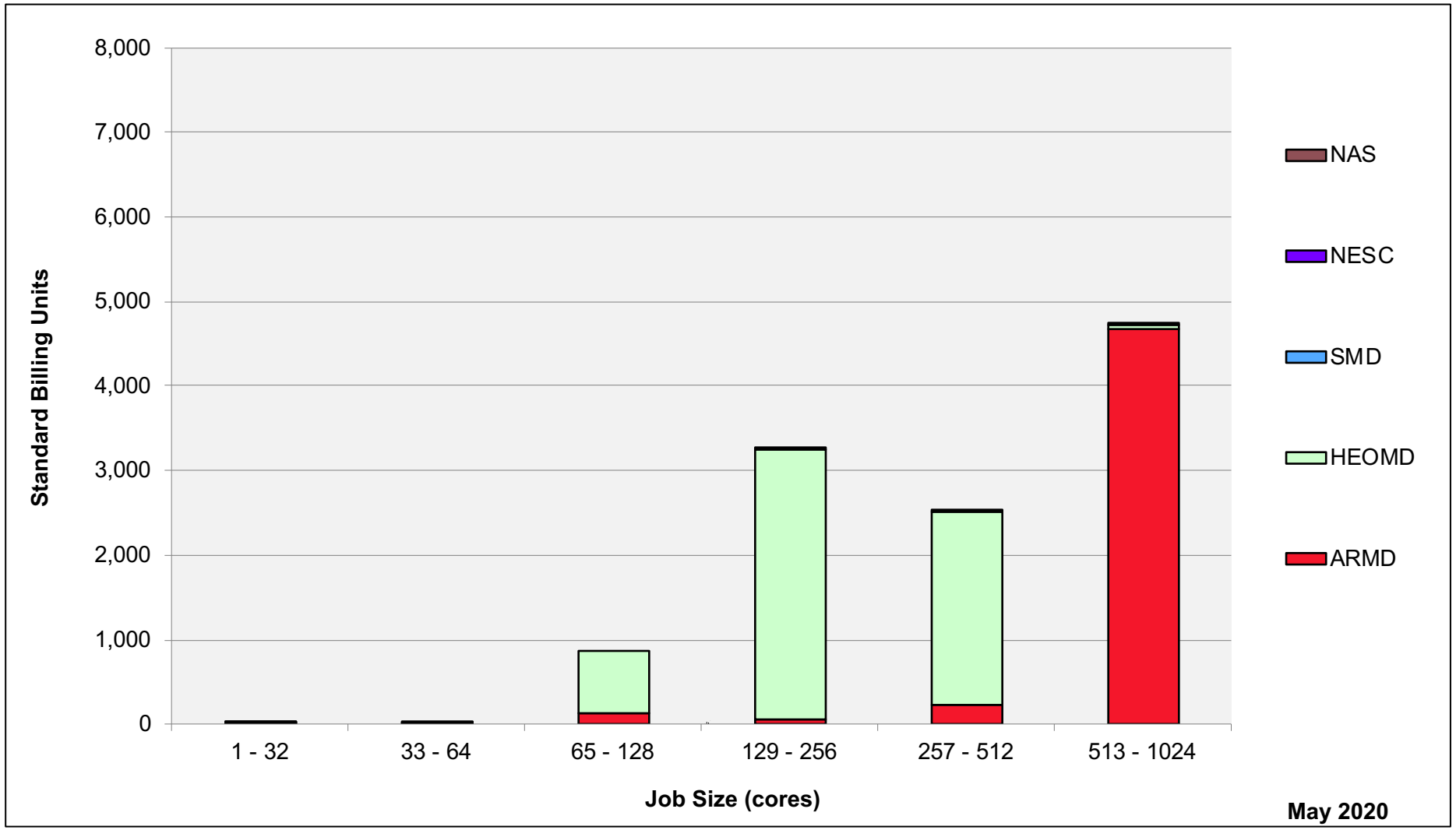
Endeavour: SBUs Reported, Normalized to 30-Day Month



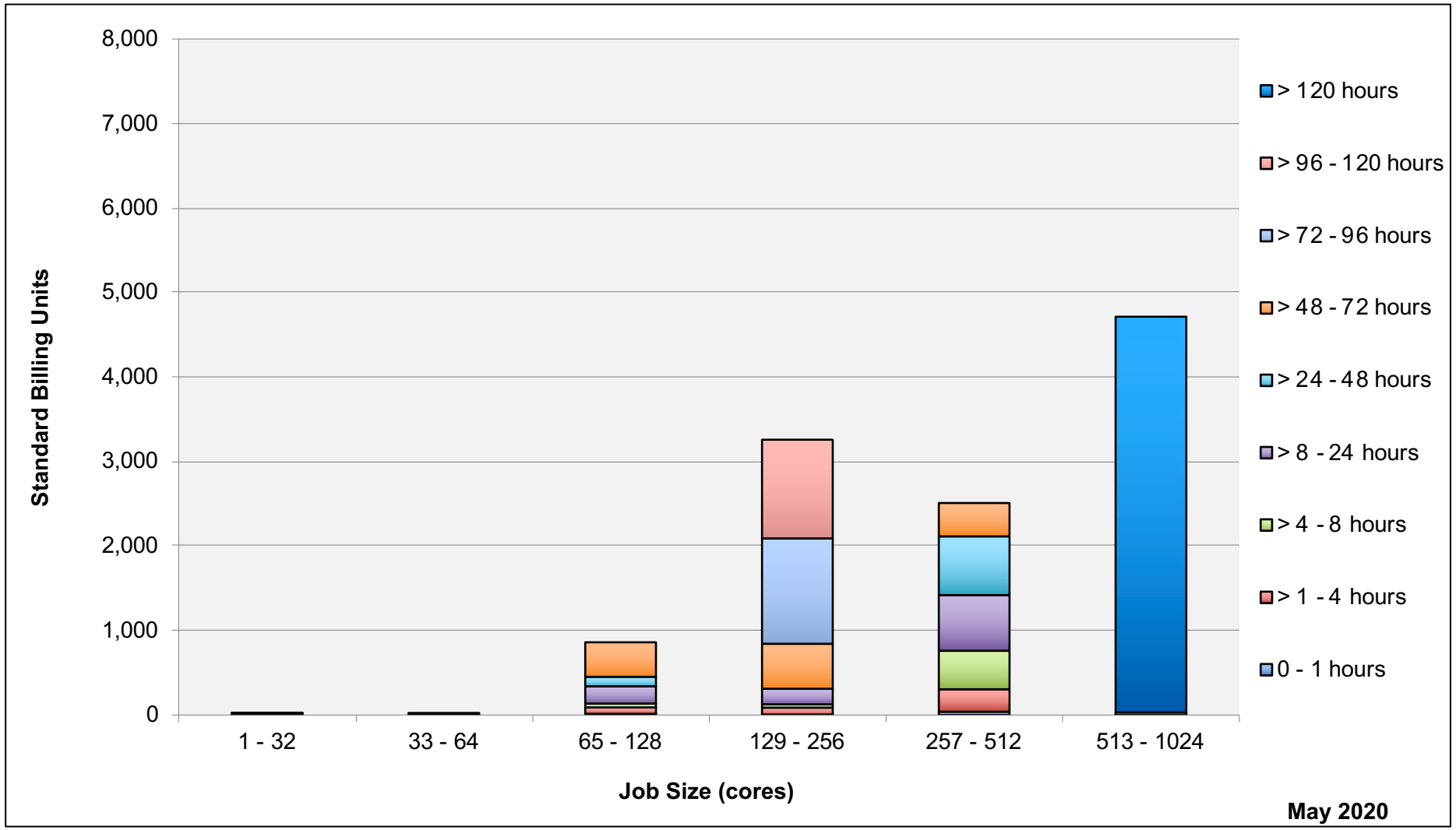
Endeavour: Monthly Utilization by Job Length



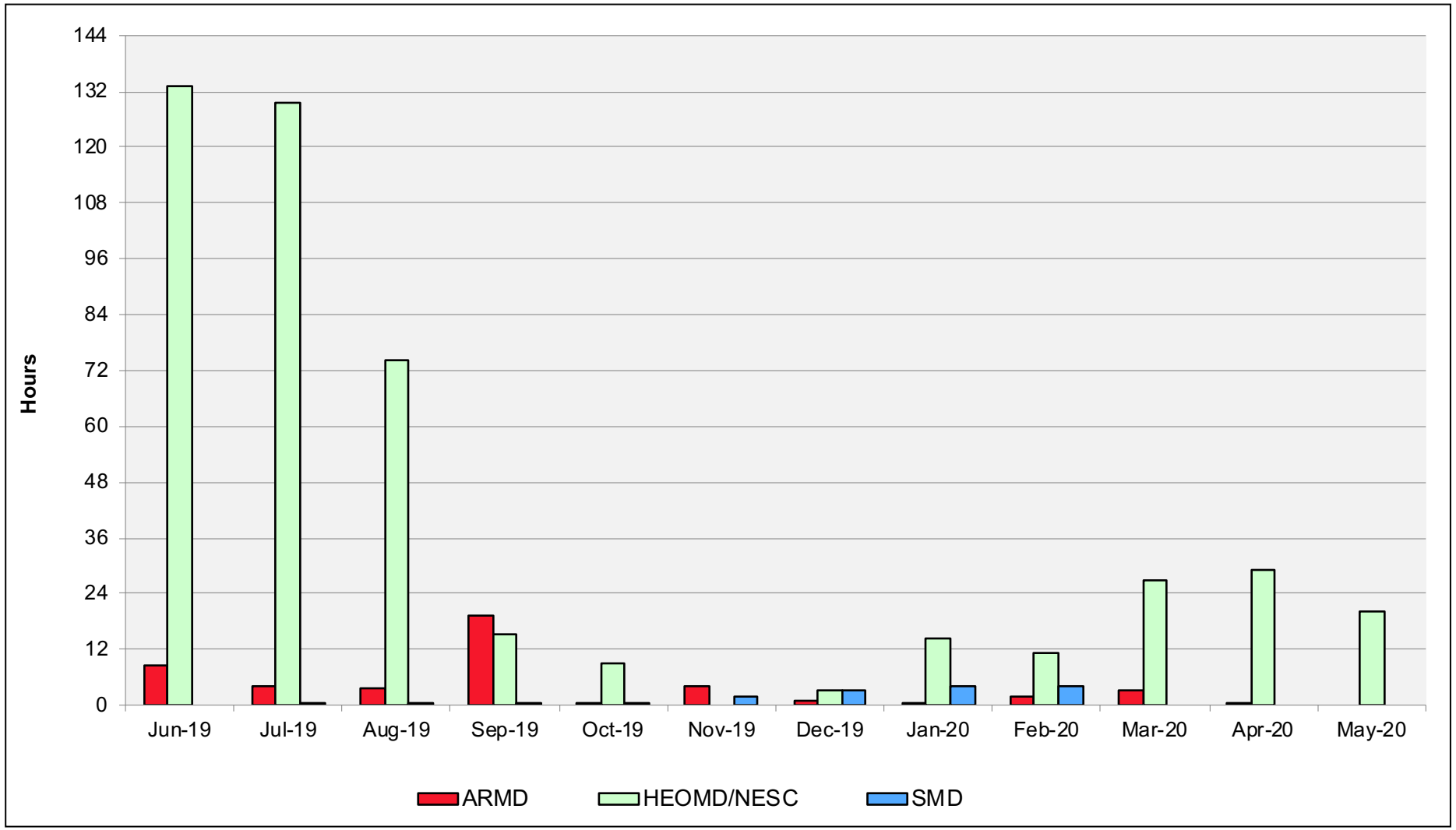
Endeavour: Monthly Utilization by Job Length



Endeavour: Monthly Utilization by Size and Length



Endeavour: Average Time to Clear All Jobs



Endeavour: Average Expansion Factor